PHYSICAL REVIEW VOLUME 175, NUMBER 1 5 NOVEMBER 1968

Rearrangement Collisions: Effect of Core Terms, Nonorthogonality, and Conservation of Particle Flux on Approximate Theories*

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(Received 27 March 1968)

Several first-order methods for rearrangement collisions are compared by applying them all to the same problem: electron-exchange scattering off the hydrogen atom. The methods considered are Born-Oppenheimer (BO); Bates-Bassel-Gerjuoy-Mittleman (BBGM); and Ochkur (O) with its modifications by Rudge and Bely. Whenever possible, they are compared with close-coupling calculations or polarized-orbital calculations. The BO approximation gives better results if the core term is retained, indicating that this inclusion helps to achieve a cancellation of errors. The BBGM first-order method is found to give reasonable integral and differential cross sections at intermediate energies but not at low energies. The methods of Ochkur and Rudge give improved integral cross sections, but at low energies the differential cross sections may be poor. The unitarization procedure of Seaton and Bely is extended to calculate exchange scattering off neutral systems but only slightly improves the Ochkur-Rudge (OR) results. None of the methods examined is satisfactory in all regards. Several other improved methods are also reviewed.

I. INTRODUCTION

In 1950, Bates, Fundaminsky, Leech, and Massey[1] made an extensive study of the Born-Oppenheimer (BO) approximation[2,3a] for the scattering of electrons by atomic systems. They concluded that BO calculations on transitions requiring electron exchange are "very poor both as regards shape and absolute magnitude" and frequently lead to cross sections which violate the conservation theorem.[3b] Further, for transitions not involving a reversal of electron spin, the exchange contribution calculated by the BO method "generally leads to gross errors at low energies"[1a] (where the electron-exchange contribution is important). These are indications that the BO approximation is poor for rearrangement processes in general.

Many workers have felt that the inadequacy of the BO approximation is due to the inclusion of core terms in the scattering amplitude. Day, Rodberg, Snow, and Sucher[4] have emphasized that, for the case of an infinitely heavy core (which is an excellent approximation for electron-exchange scattering from an atom), the exact rearrangement scattering amplitude can be written so that the matrix element of the core interaction does not contribute; i.e., if we use the exactly correct scattering wave functions to calculate the scattering amplitude, equal results are obtained whether the core is included or not. The only effect of the core is then to distort the incoming and outgoing particle waves from what they would be in the absence of particle-core interactions. Because of this they argued that the core term should not be included in the potential in the BO calculation; however, since in this approximation the incident and scattered waves are treated as undistorted, this argument is not conclusive. In other words, the plane-wave approximation can be made either before or after the core-term integration is made (in the latter case, the core interaction does not explicitly appear in the transition matrix). These are two different approximations, and it is not possible to decide in an *a priori* way which will furnish better (or more consistent) results. Some workers have argued that including the core in the BO amplitude compensates for not including distortion.[5a] We have done calculations in both the BO and the BO-minus-core (BOMC) approximations to help resolve this problem.

The prior core-interaction term would not contribute to the scattering amplitude if the initial and final wave functions of the scattered particle (which for exchange scattering is initially bound) were orthogonal. In the Born-Oppenheimer approximation, the scattered particle is represented by a plane wave. Then the necessary orthogonality holds only in the high-energy limit. Various methods have been advanced for correcting this nonorthogonality flaw in the BO approximation.[6-11] These methods explicitly or effectively establish orthogonality of initial and final states so that a constant potential will not make a contribution to the approximate rearrangement scattering amplitude. Another approach to correcting the BO amplitude was suggested by Ochkur.[12] He attempts to separate from the BO amplitude those parts which might make erroneously large contributions to the calculated scattering amplitude at low and intermediate energies by expanding the BO amplitude about its high-energy limiting form and using only the first term at all energies. Thus, those contributions that are small at high energy (where first-order theories are expected to be valid) are not allowed to become large and dominate the approximate amplitude at low energies. The Ochkur theory has been corrected by Rudge and these modified theories (O for Ochkur and OR for Ochkur-Rudge) lead to significant improvement of the calculated integral cross sections for excitation processes.[8,12-20] In all these theories, it is not clear how much of the difference from the unmodified BO approximation is due to removing parts of the core interactions, how much is due to introducing orthogonality, and, in the O and OR theories, how much is due to the rest of the changes. In this paper, we attempt to sort out some of these details.

None of these approximation schemes automatically satisfies the conservation of particle flux requirements which would be expressed by the unitarity of the scattering matrix $\underline{S}$.[21] To satisfy the unitarity requirements we employ a unitarization technique[22] involving the reactance matrix $\underline{R}$. Application of this technique to the OR method was first suggested by Bely.[23] A detailed comparison of the two methods is made in Secs. 3.4 and 3.7.

In this paper we will examine many first-order methods, applying them all to the same problem. We calculate cross sections differential in angle as a function of incident energy. For computational convenience, we consider a simple case: electron-exchange scattering off the H atom. This process is observable because it can change the value of F (the total spin of the proton–bound electron two-particle system). This $1s$-$1s$ exchange process can cause the 21-cm hyperfine transition important in radio astronomy.[24] (Spin-change cross sections may be determined in the laboratory by observing the depolarization of electron-spin-aligned atoms caused by collisions with electrons.[25]) Elastic scattering includes the exchange of identical particles if this is not accompanied by net excitation or de-excitation. The energy separations of the hydrogen hyperfine levels are a million times smaller than the translational energies of the electrons so that we will consider collisions involving only a spin change to be elastic.

The role played by the core terms and nonorthogonality in the BO expression for the amplitude will be examined. The removal of core terms in the O and OR theories will thus be separated from the other changes brought about by these theories. This is important because in more complicated cases (such as the treatment of chemical and nuclear rearrangements) it is not simple to make the Ochkur and Rudge modifications completely. We show numerically what kind of improvement can be obtained using the unitarization procedure. Although such a unitarization scheme could be applied to any approximation scheme which satisfies detailed balance, we will consider only the result of applying it to the O and Ochkur-Rudge-Bely (ORB) results. We also compare our results with the more complicated close coupling (c.c.) and polarized orbital (PO) calculations and with experiment.

In an appendix we give, for the reader's convenience, a glossary of abbreviations used for methods and approximations.

2. METHODS

2.1 Born-Oppenheimer Approximation With and Without the Core Term

Consider the exchange scattering amplitude for the process

$$e_2^- + \mathrm{H}(1s) \rightarrow e_1^- + \mathrm{H}(ns). \tag{1}$$

Let $\vec{k}_1$ and $\vec{k}_n$ denote the wave number vectors of the incident and scattered electrons, respectively. The exchange scattering amplitude for this process can be written in the BO approximation as [3c]

$$g_{1n}^{\mathrm{BO}}(\theta) = (me^2/2\pi\hbar^2)(k_n/k_1)^{\frac{1}{2}} \iint V^{\mathrm{BO}} \psi_1(r_1)\psi_n{}^*(r_2) e^{i(\vec{k}_1\cdot\vec{r}_2 - \vec{k}_n\cdot\vec{r}_1)} d\vec{r}_1 d\vec{r}_2 , \tag{2}$$

where $V^{\mathrm{BO}} = 1/r_{12} - 1/r_2,$ (3)

and ψ_1, ψ_n are bound-state wave functions for the hydrogen atom electrons. Here θ is the angle of scattering, i.e., $\theta = \arccos(\hat{k}_1 \cdot \hat{k}_n)$ and the other symbols have their usual meaning.[3c] Equations (2) and (3) are written in the prior interaction form. When the BO amplitude is calculated using approximate bound state wave functions, different results are obtained using the post and prior forms of the interaction potential.[3d] Since we know and use the exact wave functions for the H atom, the post-prior discrepancy does not appear in this case. We can also do calculations in the Day, Rodberg, Sucher, and Snow first-order approximation[4] (called BOMC), where V^{BO} is replaced by

$$V^{\mathrm{BOMC}} = 1/r_{12}; \tag{4}$$

i.e., we drop the core term. As explained in the Introduction, it is difficult to decide which of these two approximations will furnish better results in an *a priori* manner. Neither of them includes distortion. In the BOMC approximation there is no post-prior discrepancy even if approximate electronic wave functions are used for the bound states.

The integrals necessary for the calculations implied by Eqs. (2)–(4) can be evaluated using the formulas of Corinaldesi and Trainor.[26]

2.2 The Bates, Bassel-Gerjuoy, and Mittleman Methods

One method of improving the BO amplitude has been given by Bates.[6] He noted that the ambiguity in the choice of potential for the interaction matrix element is due to the nonorthogonality of the initial and final particle wave functions in this approximation. If these wave functions were orthogonal, even though not exact, the core would not contribute to the approximate scattering amplitude. Bates derived a result taking explicit account of this nonorthogonality. Similar results were derived by Bassel and Gerjuoy[27] and Mittleman.[7] They noted that although the elastic-scattering system wave function is not orthogonal to the final state system wave function, it contains no rearrangement. Hence they removed the elastic scattering from the total wave function before calculating the rearrangement amplitude. In the usual first-order approximation[28] their results agree[29a] with those of Bates. For the case of an infinitely heavy core, the core term does not contribute to the exact amplitude in their formulation. Mott and Massey, however, have shown[3e] by a variational method that the usual BO approximation should be preferred to a first-order approximation of the Bates, Bassel-Gerjuoy, and Mittleman formulation (denoted BBGM1).[29b]

The BBGM1 theory may be understood by the two-potential formula derivations of the distorted wave method.[4,27,30] The transition amplitude may be considered as due to the full interaction potential V acting on an unperturbed initial state wave or as due to some part $V-U$ of the potential acting on a wave scattered off U. Then in the BBGM1 calculation the wave distorted by U is approximated by a plane wave. Thus the BBGM1 amplitude is calculated from Eq. (2) with V^{BO} replaced by $V^{\mathrm{BBGM}}=V^{\mathrm{BO}}-U^{\mathrm{av}}$, where U^{av} is the average interaction potential in the incident channel.

Thus
$$V^{\mathrm{BBGM}}=V^{\mathrm{BO}}-\int\psi_1{}^*(r_1)V^{\mathrm{BO}}\psi_1(r_1)d\vec{\mathbf{r}}_1 \tag{5}$$
$$=1/r_{12}-\int\psi_1{}^*(r_1)(1/r_{12})\psi_1(r_1)d\vec{\mathbf{r}}_2 \tag{6}$$
$$=(1/r_{12})-(1/r_2)[1-(r_2/a_0+1)\exp(-2r_2/a_0)]. \tag{7}$$

Equation (7) shows that the BBGM treatment in this case essentially removes the singularity in the potential at $r_2=0$. Note that in obtaining Eq. (6) we regard the proton as infinitely massive (therefore stationary) during the interaction. The core term [which is of order (1/1836)] then vanishes completely. Putting (7) into (2) we obtain (in Hartree atomic units)

$$g_{11}{}^{\mathrm{BBGM1}}=g_{11}{}^{\mathrm{BO}}+96/(9+k_1{}^2)^2(1+k_1{}^2)^2+16/(9+k_1{}^2)^2(1+k_1{}^2)^2 \tag{8}$$

and

$$g_{12}{}^{\mathrm{BBGM1}}=g_{12}{}^{\mathrm{BO}}+[\sqrt{2}/(k_2{}^2+1)^2]\{4/(\tfrac{25}{4}+k_1{}^2)+10/(\tfrac{25}{4}+k_1{}^2)^2-[4(\tfrac{75}{4}-k_1{}^2)/(\tfrac{25}{4}+k_1{}^2)^3]\}. \tag{9}$$

2.3 The Ochkur and Ochkur-Rudge Methods

Recently, new modifications of the BO formula have been presented by Ochkur[12] and Rudge.[8] As mentioned above, Ochkur expanded the rearrangement scattering amplitude in inverse powers of the incident particle wave number k_1. He then suggested that one drop all terms in the expansion except the first. Thus the terms which are small at high energy (where a first-order perturbation treatment like the BO method would be expected to be valid) are neglected at all energies. The core interaction matrix element is entirely terms of this type and thus is automatically neglected. Ochkur found the first term g^{O} in the high energy expansion of the exchange amplitude for electron-atom scattering to be[12]

$$g_{1n}{}^{\mathrm{O}}(\vec{\mathbf{k}}_1,\vec{\mathbf{k}}_n)=(q^2/k_1{}^2)f_{1n}{}^{\mathrm{B}}(\vec{\mathbf{k}}_1,\vec{\mathbf{k}}_n), \tag{10}$$

where $\vec{\mathbf{q}}=\vec{\mathbf{k}}_n-\vec{\mathbf{k}}_1$ is the wave-number transfer vector so that

$$q=[k_1{}^2+k_n{}^2-2k_1k_n\cos\theta]^{1/2} \tag{11}$$

and

$$f_{1n}{}^{\mathrm{B}}(\vec{\mathbf{k}}_1,\vec{\mathbf{k}}_n)=(me^2/2\pi\hbar^2)(k_n/k_1)^{1/2}\times\iint e^{i(\vec{\mathbf{k}}_1-\vec{\mathbf{k}}_n)\cdot\vec{\mathbf{r}}_2}(1/r_{12})\psi_1(r_1)\psi_n{}^*(r_1)d\vec{\mathbf{r}}_1d\vec{\mathbf{r}}_2. \tag{12}$$

$f_{1n}{}^{\mathrm{B}}$ is the Born direct amplitude for $n\neq 1$. For elastic scattering it is only part of the Born direct amplitude. The formula (10) was first derived by Bonham.[31] The integral (12) has been evaluated for the hydrogen atom by Bethe and Massey and Mohr and is given by Corinaldesi and Trainor.[26]

An alternative derivation of Ochkur's result has been presented by Vainshtein, Presnyakov, and Sobel'man.[32] Still another derivation has been given by Vriens,[33] using a method originally suggested by Ochkur.[12]

Rudge[8] modified the O result so that the scattering amplitude can be derived in a straightforward way from a variational expression. In Rudge's treatment the initial and final wave functions of the system are explicitly orthogonal, and the scattered wave has the correct normalization at all energies. This change in normalization leads to the Ochkur-Rudge exchange amplitude[8,23,34]

$$g_{1n}{}^{\mathrm{OR}}(\vec{\mathbf{k}}_1,\vec{\mathbf{k}}_n)=\exp(i\phi_{1n})\times[(a_0q)^2/(1+a_0k_n^2)]f_{1n}{}^{\mathrm{B}}(\vec{\mathbf{k}}_1,\vec{\mathbf{k}}_n), \tag{13}$$

where
$$\phi_{1n}=2\arctan(1/a_0k_n). \tag{14}$$

2.4 The Ochkur-Rudge-Bely Method

The BO and O approximations satisfy the principle of detailed balance.[21] This is manifest in the symmetry of the S matrix.[35] Bely[23] has shown that the OR result can be corrected to satisfy detailed balance if the scattering amplitude is replaced by its absolute value. We will call this the ORB. I result, i.e.,

$$g^{\mathrm{ORB.I}}=|g^{\mathrm{OR}}| \tag{15}$$

None of these approximation schemes automatically satisfies the conservation of particle flux requirement which would be expressed in the unitarity of the scattering matrix $\underline{S}$.[21] Violation of the conservation theorem can be avoided by using a unitarization technique[22,36,37] involving the reactance matrix $\underline{R}$.[38] This is a powerful technique because the real and symmetric R matrix has the property that the S matrix calculated from any set of approximate R matrix elements is necessarily unitary.[3f] Percival,[36] Seaton and co-workers,[22,37] and Somerville[39] have used this fact to correct the Born approximation for direct scattering and Bernstein, Dalgarno, Massey, and Percival[40] have employed a similar correction. Bely[23] has used the reactance matrix technique to correct the ORB. I result for rearrangement scattering. The corrected version is called the ORB. II approximation.

(We will also apply the correction to the O approximation, which may also be called O. I, and call the unitarized result the O. II method.)

To perform the unitarization we first expand[41] $g(\theta)$ in partial waves to obtain the weak coupling T matrix. For s states,

$$g_{1n}{}^{I}(\theta) = \frac{1}{2ia_0k_1} \sum_{l=0}^{\infty} (2l+1) T_{1n}{}^{I,l,\mathrm{ex}} P_l(\cos\theta). \quad (16)$$

We do the required expansion integrals analytically[42] but in more complicated cases they can be done numerically.

This weak coupling T matrix (called $\underline{T}^I$) should be and is a pure imaginary number and is related to the R matrix by

$$\underline{T}^I = 2i\underline{R} \ . \quad (17)$$

From the R matrix we obtain a unitary S matrix

$$\underline{S} = (\underline{1} + i\underline{R})/(\underline{1} - i\underline{R}) \quad (18)$$

and finally a corrected T matrix $\underline{T}^{\mathrm{II}}$ by

$$\underline{T}^{\mathrm{II}} = \underline{S} - \underline{1} \ . \quad (19)$$

In order for $\underline{T}^{\mathrm{I}}$ to be pure imaginary we must have g pure real. We obtain from the Ochkur approximation (O.I) a corrected O.II T matrix and amplitude. From the ORB. I result we obtain the corrected ORB. II T matrix and amplitude. Although the ORB. I result at first appears worse than the OR result (because it neglects the complex phase), Bely[23] has shown that no real improvement is lost in the procedure described by Eq. (15). [This last statement applies only when there is no interfering direct process occurring (see Eqs. (32) and Section 3.4.)].

To make calculations according to (18) for the 1s → 1s and 1s → 2s processes, we need also to know the 2s → 2s amplitude. It can be shown that for elastic scattering with spin flip from the 2s state at incident wave number k_2 we have

$$g_{22}{}^{\mathrm{OR}} = \frac{2}{(k_2 - i/2)^2} \int \psi_2{}^2(r_1) e^{i\vec{q}\cdot\vec{r}_1} d\vec{r}_1 \quad (20)$$

$$= \frac{2}{(k_2 - i/2)^2} \left[\frac{1 - 3q^2 + 2q^4}{(1+q^2)^4} \right] \quad (21)$$

$$g_{22}{}^{O} = [\,(k_2 - i/2)^2/k_2{}^2] g_{22}{}^{\mathrm{OR}} \quad (22)$$

and

$$g_{22}{}^{\mathrm{ORB.\,I}} = \frac{2(1 - 3q^2 + 2q^4)}{(k_2{}^2 + \frac{1}{4})(1+q^2)^4} , \quad (23)$$

where $\psi_2(r_1)$ is the bound-state wave function of electron 1 bound to the proton in a 2s state. Again, the results are given in Hartree atomic units.

2.5 The Close-Coupling Method

Whenever possible, we compare our results with the exchange scattering amplitude from the close-coupling approximation calculations of Burke and Schey[43] and Burke, Schey, and Smith[44] (BSS). Calculations by the more accurate correlation method are not yet available for all the cases considered here. The BSS c. c. calculations include three states of the H atom: 1s, 2s, and 2p. In general,

$$g_{1n}(\theta) = \tfrac{1}{2}[A_{1n}(\theta) - A_{1n}{}^{1}(\theta)], \quad (24)$$

where $A_{1n}{}^0$ and $A_{1n}{}^1$ are the singlet ($S = 0$) and triplet ($S = 1$) scattering amplitudes, respectively (S is the total spin of the two-electron system). Expanding in partial waves, we have (for s states)[45]

$$A_{1n}{}^{S}(\theta) = \frac{1}{2ia_0k_1} \sum_{l=0}^{\infty} (2l+1) T_{1n}{}^{lS} P_l(\cos\theta) \ . \quad (25)$$

For elastic scattering below the threshold for the first excitation process (10.2 eV), the phase shifts are real and we have

$$T_{11}{}^{lS} = e^{2i\eta_l{}^S} - 1 \ , \quad (26)$$

where $\eta_l{}^S$ is the phase shift. In the other cases the T matrix is calculated from the R matrix by

$$\underline{T}^{lS} = 2i\underline{R}^{lS}/(\underline{1} - i\underline{R}^{lS}) \ . \quad (27)$$

Equation (27) is, of course, equivalent to Eqs. (18) and (19). We calculated the T matrix from published phase shifts[43] and R matrix elements,[44] and then used Eqs. (24) and (25) to obtain the exchage amplitudes.

For purposes of comparison, we also computed exchange elastic cross sections from the phase shifts of Temkin and Lamkin.[46] These were obtained using Eqs. (24)–(26) as above.

2.6 Integral Cross Sections

The methods outlined above all lead to the exchange differential cross sections

$$I^{\mathrm{ex}}(\theta) = |g(\theta)|^2 \ . \quad (28)$$

We obtain the integral cross sections by a 49-point Weddle's Rule[47] integration (unequal steps) over the differential cross section using

$$Q_{mn}{}^{\mathrm{ex}} = 2\pi \int I_{mn}{}^{\mathrm{ex}}(\theta) \sin\theta \, d\theta \ . \quad (29)$$

This was checked by a 61-point quadrature and also by the formula

$$Q_{11}{}^{\mathrm{ex}} = \frac{\pi}{k_1{}^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\eta_l{}^0 - \eta_l{}^1) \quad (30)$$

for elastic scattering below the first threshold and by the formula[48]

$$Q_{mn}{}^{\mathrm{ex}} = \frac{\pi}{k_m{}^2} \sum_{l=0}^{\infty} (2l+1) \left| T_{mn}{}^{l,\mathrm{ex}} \right|^2 \quad (31)$$

in the other cases. The integral cross sections computed by the two methods in general agreed to six decimal places.

2.7 Direct Scattering

Because the rearrangement we are considering is an exchange of identical particles, the amplitude can interfere wave mechanically with the corresponding direct scattering process. We must take the correct linear combination of amplitudes to exchange degenerate states in order to obtain the total probability for the process

$$e^- + \mathrm{H}(m) \to e^- + \mathrm{H}(n),$$

where now the electrons are treated as indistinguishable. We find that the total differential cross section is

$$I_{mn}^{\mathrm{t}}(\theta) = I_{mn}^{\mathrm{d}}(\theta) + I_{mn}^{\mathrm{ex}}(\theta) + I_{mn}^{\mathrm{int}}(\theta), \tag{32}$$

where $I^{\mathrm{d}}(\theta) = |f(\theta)|^2$ (32a)

is the direct differential cross section, $f(\theta)$ is the direct scattering amplitude, $I^{\mathrm{ex}}(\theta)$ is the exchange differential cross section, and

$$I^{\mathrm{int}}(\theta) = -\operatorname{Re}[f(\theta)g^*(\theta)] \tag{32b}$$

is the interference contribution. The exchange scattering is sometimes called spin-flip scattering.

2.8 Experimental Cross Sections

Three sets of "experimental" spin-flip cross sections for the 1*s*-2*s* excitation were obtained as follows. Lichten and Schulz[49] measured the ratio of Q_{12}^{ex} to Q_{12}^{tot}. (The total cross section Q_{12}^{tot} includes both direct and exchange scattering.) They claim for their ratio an accuracy of 5% for energies within a few eV of threshold and 8% elsewhere. Since there is still no universal agreement on the absolute magnitude of Q_{12}^{tot}, the Lichten-Schulz (LS) ratio was combined with three different sets of data. Stebbings, Fite, Hummer, and Brackman (SFHB)[50] normalized their data for Q_{12}^{tot} by using their experimental $Q_{1s\text{-}2s}'/(Q_{1s\text{-}2s}' + Q_{1s\text{-}2p})$ and the Born approximation at 200 eV to normalize their experimental $Q_{1s\text{-}2p}$. The $Q_{1s\text{-}2s}'$ so obtained is the total cross section for production of 2*s* atoms, including the contribution due to radiative decay from higher levels excited by electron impact. We retained their normalization procedure but use the

TABLE I. The scattering amplitude for 1*s*-1*s* exchange scattering (in a_0).

θ	E	g^{BO}	g^{BOMC}	g^{BBGM1}	g^{O}	$\lvert g^{\mathrm{OR}}\rvert$	ϕ^{OR}	$\lvert g^{\mathrm{BS}}\rvert$
15°	4 eV	-1.815	5.570	-0.123	6.735	1.530	123	
	8	-0.389	3.606	0.686	3.334	1.235	105	
	12	0.166	2.566	0.901	2.201	1.031	94	
	16	0.394	1.947	0.922	1.634	0.883	85	
	20	0.484	1.545	0.878	1.295	0.771	79	
	28	0.508	1.068	0.747	0.907	0.610	70	
	36	0.470	0.801	0.627	0.692	0.502	63	
	44	0.422	0.633	0.530	0.556	0.424	58	
	60	0.335	0.436	0.394	0.392	0.320	51	
	80	0.257	0.306	0.289	0.281	0.240	45	
	100	0.204	0.231	0.223	0.215	0.189	40	
	150	0.127	0.136	0.134	0.129	0.118	34	
	300	0.048	0.050	0.049	0.047	0.046	24	
	500	0.021	0.021	0.021	0.021	0.020	19	
18°	0.01 Ry	-5.761	9.769	-2.861	199.902	1.979	169	2.185
	0.1	-4.011	8.010	-1.600	19.902	1.809	145	0.982
	0.3	-1.782	5.501	-0.107	6.570	1.516	123	0.276
	0.5	-0.699	4.402	0.522	3.904	1.301	109	0.629
	0.7	-0.137	3.119	0.787	2.762	1.137	100	0.583
	1.0	0.261	2.261	0.901	1.906	0.953	90	0.550
	1.44	0.455	1.557	0.861	1.296	0.765	80	0.641
	2.25	0.476	0.942	0.682	0.799	0.553	67	0.588
	4.00	0.340	0.468	0.412	0.415	0.332	53	0.369
85°	4.00 Ry	-0.021	0.107	0.051	0.063	0.050	53	0.072
140°	4.00 Ry	-0.070	0.058	0.002	0.024	0.019	53	0.059
18°	11 eV	0.049	2.754	0.853	2.379	1.063	96	
60°	11 eV	-0.450	2.255	0.354	1.712	0.765	96	
120°	11 eV	-1.076	1.629	-0.272	0.959	0.429	96	
170°	11 eV	-1.260	1.445	-0.456	0.761	0.340	96	

TABLE II. The scattering amplitude for 1*s*-2*s* exchange scattering at 45° (in a_0)

E (eV)	g^{BO}	g^{BOMC}	g^{BBGM1}	g^{O}	$\lvert g^{OR}\rvert$	ϕ^{OR}
12	-0.5950	0.7592	-0.4558	0.1970	0.1535	140
16	-0.3489	0.6339	-0.2218	0.1936	0.1596	114
20	-0.1660	0.4936	-0.0622	0.1779	0.1521	99
24	-0.0633	0.3899	0.0209	0.1604	0.1405	90
28	0.0074	0.3144	0.0615	0.1434	0.1279	82
36	0.0384	0.2157	0.0858	0.1136	0.1038	72
44	0.0487	0.1560	0.0827	0.0902	0.0837	65
52	0.0476	0.1172	0.0728	0.0723	0.0679	59
60	0.0430	0.0906	0.0622	0.0586	0.0555	55
80	0.0304	0.0522	0.0410	0.0364	0.0349	48
100	0.0211	0.0329	0.0277	0.0240	0.0232	43
150	0.0095	0.0132	0.0120	0.0103	0.0100	35
300	0.0018	0.0023	0.0022	0.0019	0.0019	24
500	0.0005	0.0006	0.0006	0.0005	0.0005	19

recent calculations of Morrison and Rudge[15] to recorrect for the cascade. The corrected result is called Q_{12}^{SFHB}. Hils, Kleinpoppen, and Koschmeider (HKK)[51] normalized their data to the Born approximation for Q_{12}^{tot} at 200 eV. Their result is called Q_{12}^{HKK}. Burke, Taylor, and Ormande (BTO)[52] suggested that the Lichten-Schulz Q_{12}^{tot} measurements be normalized to correlation method calculations of Taylor and Burke[53] in the region 10–11 eV. This gives a third experimental curve (called $Q_{12}^{LS\text{-}BTO}$). There have been no experiments on the elastic exchange scattering from the hydrogen atom.

3. RESULTS AND DISCUSSION

3.1 Contribution of the Core to the BO Amplitude

Although the spin-flip differential and integral cross sections depend only on $|g|^2$, the sign, or complex phase factor, of g is important in calculating total cross sections [see Eqs. (32)]. Also, since contributions to g from the rearrangement term $1/r_{12}$ and the core term $-1/r_2$ are of opposite sign, a study of g including the sign can be informative in discerning the effect of the core term. Tables I–III give values of g computed in the various nonunitarized approximations at various energies and angles. These are typical results – the results for other angles are qualitatively similar. The values of $|g|$ for exchange elastic scattering which we computed from three-state close-coupling approximation results[43,44] are also presented where available. At energies below 0.85 Ry these are very accurate[54] and serve as a standard for comparison. Comparing the BO and BOMC amplitudes we see that the core term dominates the BO scattering amplitude at low energies. This fact had been previously conjectured for electron scattering.[8,20] However, merely dropping the core term (as suggested by Day *et al.*) leads to even worse numerical agreement with the accurate calculations. Bates, Fundaminsky, and Massey[1a] and Massey and Burhop[55a] have cautioned that keeping the core term was probably necessary for a partial cancellation of errors in the approximate BO theory, and Bates[56] pointed out that the BOMC approximation is especially bad at low energies; but we have not found any examples in the literature (other than the ones given here) where this has been shown by a direct comparison of the

TABLE III. The scattering amplitude for 1*s*-2*s* exchange scattering at 120° (in a_0).

E (eV)	g^{BO}	g^{BOMC}	$\lvert g^{OR}\rvert$	ϕ^{OR}
12	-0.5499	0.8043	0.1798	140
16	-0.3817	0.6010	0.1500	114
22	-0.2562	0.4035	0.1038	99
24	-0:1783	0.2749	0.0780	90
28	-0.1289	0.1929	0.0573	82
36	-0.0737	0.1036	0.0331	72
40	-0.0577	0.0788	0.0259	68
50	-0.0339	0.0432	0.0151	61
100	-0.0059	0.0059	0.0024	43
250	-0.0005	0.0004	0.0002	27
500	-0.0000_7	0.0000_4	0.0000_2	19

TABLE IV. Total differential cross section $I^{t}_{1n}(\theta)$ calculated using the Born approximation for $f(\theta)$. $E=1.0$ Ry. Cross sections in a_0^2.

n	θ	BOMC	BO	O	OR	BBGM1
1s	30°	7.370	0.976	5.505	1.596	2.152
	60°	4.876	0.403	3.078	0.928	0.964
	90°	3.103	0.325	1.593	0.506	0.343
	120°	2.160	0.491	0.921	0.308	0.154
2s	30°	0.364	0.720	0.146	0.245	0.528
	60°	0.432	0.455	0.071	0.151	0.301
	90°	0.478	0.336	0.046	0.091	0.201
	120°	0.476	0.312	0.036	0.059	0.179

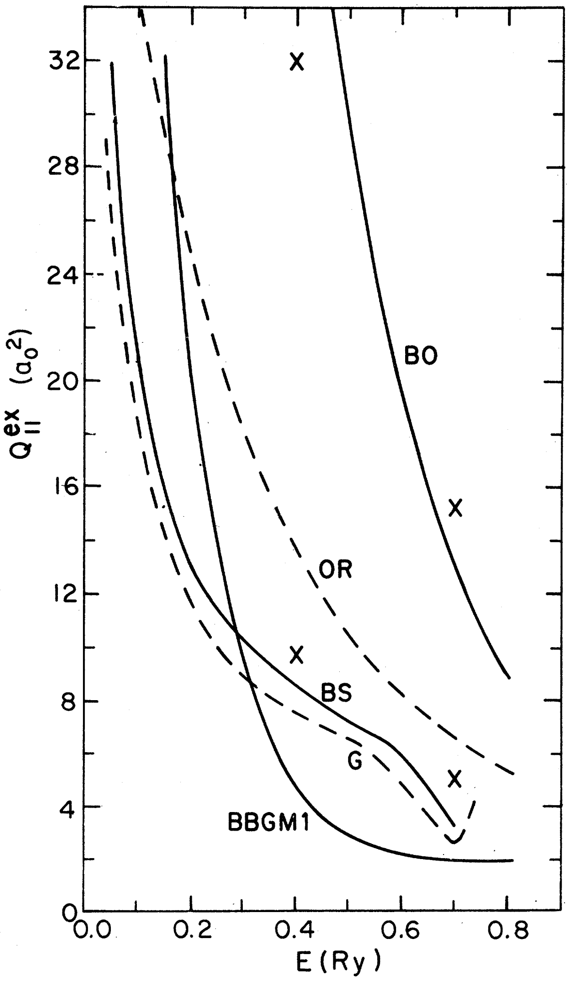

FIG. 1. Integral exchange elastic cross sections (in a_0^2) for electron-hydrogen scattering in several approximate theories and from the accurate calculations of Burke and Schey (BS) and Gailitis (G). The small ×'s show results from the unitarized calculations discussed in Sec. 3.7. The two lowest ×'s are ORB. II results and the two higher ×'s are O. II results.

two methods for the same process. Clearly neither the BO nor the BOMC result is useful at low energies. Similar considerations apply to the 1s-2s amplitudes (Tables II, III) where the BO and BOMC results are much larger than the approximately correct[8] OR results. To further emphasize the unsuitability of the BOMC result we have computed a few values of $I^t(\theta)$ using Eqs. (32) and the Born approximation[26] for f. These are presented in Table IV for the several methods of computing g.

At very high energies, the contribution of the core term is smaller. In the examples considered here, the difference between the BOMC and the BO integral cross sections is about 10% at 300 eV and 1% at 1000 eV.

The results discussed in this section indicate that merely dropping the core term (as suggested by Kang and Sucher[4]) worsens the results. The next section discusses the BBGM1 method, which is a more consistent way to correct the BO amplitude.

3.2 The Modified Born Approximation of Bates, Bassel and Gerjuoy, and Mittleman

As seen in Tables I-IV, the BBGM1 results are better than the BO and BOMC ones. This indicates that the "effective orthogonality" of the approximation is partially successful in removing spurious core contributions and in leading to a more consistent treatment. Figure 1 compares the BO, OR, and BBGM1 cross sections for the low-energy exchange elastic scattering with the accurate results of Burke and Schey and the very accurate variational results of Gailitis.[57] (The BOMC and O results are much too high in this energy range. They are, respectively, 10–23 times and 5–120 times larger than the OR result in the range shown.) Figure 2 compares the integral 1s-2s exchange cross sections computed in the various approximations with the BTO and SFHB experimental results (the HKK experiment gives results about 0.7 times the SFHB results). These figures show that the BBGM1 result is a considerable improvement over the BO approximation but is not accurate enough for useful quantitative predictions in all cases.

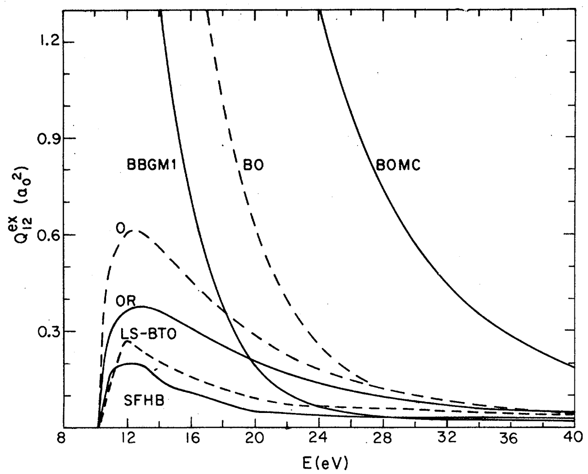

FIG. 2. Integral exchange cross sections (in a_0^2) for the $1s$-$2s$ excitation of hydrogen by electrons in several approximate theories and from experiment (LS and SFHB). The rise of the BBGM1, BO, and BOMC approximate curves is not shown. The BO result is not drawn for energies above 27 eV. In that region it drops below the O and OR results. The failure of the BBGM1 theory at low energies here is similar to the failure of the E1 approximation at low energies for He exchange excitation (cf. Figs. 1 and 2 of Ref. 18).

There are other methods in use which are closely related to the BBGM1 result. Feenberg[58] derived an expression for the exchange amplitude by successive approximations solution for the scattered wave function using a wave scattered off U^{av} as a first approximation. He then made a first-order approximation and found that the BO approximation did not include all terms first order in the interaction potential. Bell and Moiseiwitsch[59] rederived this result using the method of Bates.[6] They called their result the first-order exchange ($E1$) method. For elastic scattering

$$g_{nn}^{E1} = g_{nn}^{\mathrm{BBGM1}}, \tag{33}$$

but for exchange excitation the $E1$ result contains one more term. This corresponds to using in Eq. (2) the potential

$$V_{1n}^{E1} = V^{\mathrm{BBGM}} - \int \psi_n^*(r_1) V^{\mathrm{BO}} \psi_1(r_1) d\tau_1. \tag{34}$$

Bell, Eissa, and Moiseiwitsch[60] noted that this term is small in the case of atomic hydrogen excitation to the $2s$ and $2p$ states except just above threshold.[59,61] Consequently, they neglected this term in their calculation of exchange scattering off He.[60] Mittleman[7] has developed a whole series of approximations in which some of the nonrearrangement part of the wave function is projected out before the rearrangement scattering amplitude is calculated. If only the direct elastic scattering is removed the result is the BBGM approximation used above. If the direct elastic scattering and direct excitation to the state n are removed, and the exchange excitation to state n is calculated in first-order approximation, the result is the $E1$ approximation.

The BBGM1 and $E1$ approximations are interesting because their application to complicated problems involving general potentials is straightforward Indeed the BBGM1 method has been very instructive in considerations of the charge-transfer process

$$A^+ + B \rightarrow A + B^+. \tag{35}$$

In the electron scattering case the core term is replaced by one similar in appearance [compare Eqs. (3) and (7)] but different in origin. In the BBGM1 treatment of the electron-capture reaction

$$\mathrm{H}^+ + \mathrm{H} \rightarrow \mathrm{H} + \mathrm{H}^+, \tag{36}$$

the same is true of the term representing the interaction of the two positive nuclei (this is not a core term in the sense of Day *et al.*[4]). The appearance of these nuclear interaction terms in the BO interaction potential for reactions (1) and (36) was regarded as somewhat unphysical, and it was not completely understood why their inclusion improved agreement with experiment.[56,62,63] However, the "unphysical" term in the BO potential and the term in the BBGM1 potential would not be so similar if the nucleus involved had a larger charge [as in (35) with B a hydrogenic atom of nuclear charge Z greater than 1] or if the interactions were not both of the same (here coulombic) form.[27] That the approximate correctness of the BO amplitude for (1) and (36) is an accident related to the proton and electron having the same charge is substantiated by the worsening of the BO approximation for the process[63]

$$\mathrm{He}^{++} + \mathrm{H} \rightarrow \mathrm{He}^+ + \mathrm{H}^+. \tag{37}$$

In the final state of reaction (37) there is a proton and a hydrogenic atom of charge Z greater than one. Jackson showed that the unphysical term in the BO approximation for (36) is canceled by an identical term in the second Born approximation but that this cancellation does not occur for (37). It is expected that the origin of terms in the BBGM1 approximation is essentially correct, and the BBGM1 approximation should be applicable not only to (1) and (36) but also to (37) and a wide variety of other reactions.

3.3 The Modified Born Approximation of Ochkur and Rudge

We have seen that while the BBGM1 and $E1$ approximations are a great improvement on the BO approximation, they sometimes still overestimate the cross sections at low energies. The methods of Ochkur and Rudge are an attempt to correctly extrapolate the BO amplitude to low energies by retaining at all energies only the term in an expansion of the matrix element in powers of $(1/k)$ which is largest at high energies. The O approximation may be considered just as an OR approximation with improper normalization of the wave function. Using a trial function whose high-energy limit is suggested by the O result but which has the correct asymptotic form at all energies, the OR result can be derived either with[8] or without[64] a variational principle. Thus in the high-energy limit the OR, O, and BO results are identical. For electron

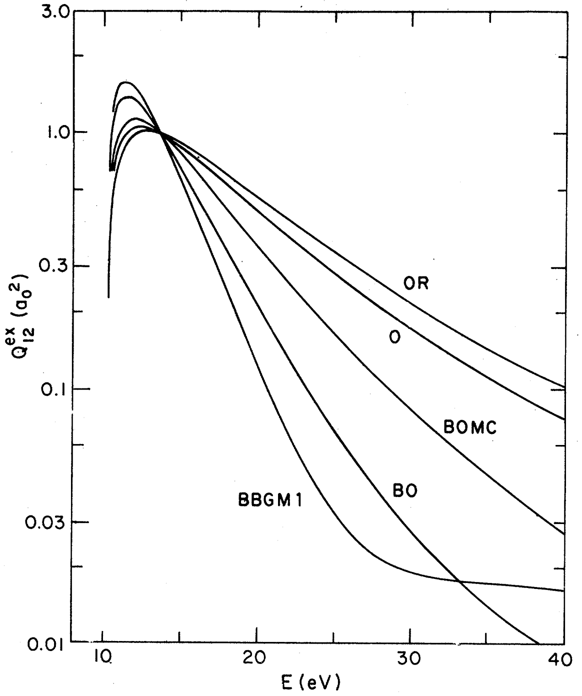

FIG. 3. Integral exchange cross sections (in a_0^2) for the $1s$-$2s$ excitation of hydrogen by electrons in several approximate theories. This semilog plot illustrates the shapes of the cross sections; when two curves are parallel, the cross section curves have the same shape. Data are all normalized at 13.605 eV for this plot. At the far left, the order of the cross sections (from top down) is: BBGM1, BO, BOMC, O, and OR. The initial rise of each cross section is not shown. Four of the shapes agree approximately with the shape of the experimental curves (not shown). The BBGM1 shape is poor at these energies.

scattering from atoms, the matrix element of the core interaction vanishes very rapidly at high energy, and the BOMC and BBGM1 results also approach the BO approximation. It should be mentioned, however, that this is not always the case. For Reaction (35) the term representing the interaction of the two nuclei contributes appreciably to the BO amplitude at all energies[3e] and the BO and BBGM1 results are not identical at high energy. In fact Q^{BBGM1} tends to the Brinkman-Kramers[65] result Q^{BK} – which is obtained by omitting the nucleus-nucleus interaction from the BO approximation.[66] In the high-energy limit for the Reaction (36), $Q^{\mathrm{BK}} = 1.51 Q^{\mathrm{BO}}$, but this limit is attained very slowly. At 1 MeV,[68] $Q^{\mathrm{BK}} = 2.70 Q^{\mathrm{BO}}$ and $Q^{\mathrm{BBGM1}} = 1.98 Q^{\mathrm{BO}}$.

Table I shows that the O approximation fails badly for low-energy elastic scattering. This was expected from the comments of Morrison and Rudge,[15] who noted in comparing the O and OR amplitudes that the former would not give reliable results for any transition in which the energy separation is small compared with the ionization energy. This particular shortcoming of the O approximation is also demonstrated in the cross section for the $2^3S \rightarrow 2^1P$ excitation of He as calculated by Ochkur and Brattsev.[69] If one assumes only the s and p partial waves can contribute this calculated cross section violates the conservation theorem[3b] by factors of 364 and 146 at 2 and 4 eV, respectively. Another example is the $2^3S \rightarrow 2^1S$ process in He, as discussed by Morrison and Rudge[18] and Beigman and Vainshtein.[10]

Figures 2 and 3 and previous calculations by others[8,15,18,20] show that the OR approximation for exchange-excitation processes gives a reliable integral cross-section curve with close to the correct magnitude and shape. For the elastic scattering the agreement is worse. For elastic scattering the Born approximation has long been considered inaccurate[70] and the new modifications may not have completely corrected this.[8] A possible explanation of this failing is that a first-order perturbation approximation to the scattering amplitude does not include all the important interactions in the low-energy region. In this energy range, the distortion effects of the long-range polarization potential are important but are not included in the usual first-order theory. This interaction may affect the elastic scattering so strongly that first-order methods which neglect it do not work well.

3.4 Complex Nature of the Scattering Amplitude

The exact scattering amplitude g^e is a complex number, i.e., $g^e = |g^e| \exp(i\phi^e)$. The phase ϕ of the exchange scattering amplitude does not affect the exchange cross section but does enter into the term for the interference of direct and exchange scattering [see Eqs. (32)]. The phase is also important in determining the interference between scattering from different centers as in high-energy electron scattering from a molecule with two or more nuclei.[71,72] Further, a calculation predicts zero spin polarization of the scattered electron unless at least one of f and g is complex.[73] It is well known that the scattering amplitude cannot be consistent with conservation of particle flux unless it is complex.[74] This complexity, however, is a necessary but not a sufficient criterion. The complex result of Bely (ORB. II) does, however, automatically satisfy the conservation theorems. The complex O.II expression or any other unitarized expression is also satisfactory in this regard. Table V illustrates the complex nature of some of these amplitudes. There is no apparent correlation between the phases of the close-coupling exchange amplitudes and the phases of the unitarized first-order approximations. In general, though, the OR result is closer to 180° when the BO and BBGM1 results are negative and closer to 0° when they are positive. The phase of the OR result has previously been criticized by Bely.[23] The comparison in Table V, however, shows that none of the first-order methods considered here gives the phase of the exchange scattering amplitude in agreement with BSS.

3.5 Angular Distrubution at Intermediate Energies

The literature has very little discussion of angular distributions of scattered particles as predicted by first-order theories of rearrangement. This is because there is hardly any experimental

TABLE V. Scattering amplitudes.

n	E (Ry)	θ (deg)	$\lvert g^{\mathrm{O.II}}\rvert$	ϕ^{OR}	$\lvert g^{\mathrm{OR}}\rvert$	ϕ^{OR}	$\lvert g^{\mathrm{ORB.\,II}}\rvert$	$\phi^{\mathrm{ORB.\,II}}$	$\lvert g^{\mathrm{BSS}}\rvert$	ϕ^{BSS}	$\lvert g^{\mathrm{BBGM1}}\rvert$	ϕ^{BBGM1}
1s	0.4	42	2.1356[a]	45.9	1.292	115.4	1.029[a]	26.0	0.4174[c]	-91.6	0.0702	0.0
1s	0.4	80	1.5307[a]	63.4	1.052	115.4	0.8863[a]	31.9	0.5513[c]	-31.2	0.3973	180.0
1s	1.0	42	1.2121[a]	30.4	0.7853	90.0	0.7196[a]	18.6	0.6895[b, d]	-116.9	0.6367	0.0
			1.1920[b]	30.5			0.7034[b]	19.8	0.5088[c]	-131.1		
1s	1.0	80	0.7189[a]	46.4	0.5007	90.0	0.4497[a]	27.2	0.5210[b, e]	-104.9	0.1581	0.0
			0.7001[b]	47.0			0.4360[b]	29.4	0.4096[c]	-92.2		
2s	1.0	42	0.1204[b]	75.9	0.1548	126.9	0.1313[b]	42.5	0.2199[c]	49.5	0.3711	180.0
2s	1.0	60	0.1365[b]	68.5	0.1778	126.9	0.1507[b]	37.7	0.1773[c]	83.7	0.3368	180.0
2s	1.0	80	0.1480[b]	6[illegible].3	0.1872	126.9	0.1593[b]	36.4	0.1539[c]	130.3	0.3228	180.0
2s	1.0	100	0.1448[b]	65.4	0.1838	126.9	0.1568[b]	37.4	0.1019[c]	156.8	0.3296	180.0
2s	1.00	120	0.1387[b]	69.3	0.1750	126.9	0.1495[b]	39.3	0.0728[c]	[illegible]22.7	0.3464	180.0
2s	1.44	80	0.1438[b]	36.6	0.1514	100.6	0.1376[b]	24.5	0.0747[c]	-158.9	0.0878	180.0
2s	2.25	80	0.0841[b]	24.2	0.0825	78.5	0.0786[b]	17.8	0.0743[c]	-100.8	0.0146	0.0
2s	4.00	80	0.0279[b]	14.9	0.027[illegible]	58.0	0.0265[b]	12.3	0.0296[c]	-78.5	0.0189	0.0

[a] 1×1. [b] 2×2. [c] 4×4. [d] 1×1 was 0.8035. [e] 1×1 was 0.5500.

data available. One case for which comparison is possible is the electron impact exchange excitation of the He 2^3S state. The differential cross sections predicted by the O and OR methods (the O, OR, and ORB.I methods predict – except for normalization – the same angular distributions) are peaked off zero degrees at all energies up to 95 eV.[75a] This agreed with the experiments of Ehrhardt and Willman[76] at 22–24 eV but disagreed with the 56.5-eV experimental results at 5–50° of Simpson, Menendez, and Mielczarek.[77] Vriens, Simpson, and Mielczarek[78] studied experimentally the angular distribution from 5 to 15° in the energy range 100–225 eV. They also found the differential cross section predicted by the O approximation disagreed strongly with experiment. They could not test the validity of the O approximation at larger angles. Miller and Krauss[79] calculated the BOMC differential cross section from 0 to 60° for comparison with these results. They found that at these high energies and these angles the BOMC and O results agreed and hence the BOMC also disagreed with experiment. A second case for which comparison is possible is excitation of the $b^3\Sigma_u^+$ state of H_2. The angular distribution for excitation scattering to this state at 35–60 eV is peaked off 0° and agrees with the OR result, but at lower energies it disagrees.[75] There has been no previous report of the BBGM1 angular distributions.

The electron scattering off atomic hydrogen presents an opportunity to test the various methods because they can be compared with close-coupling calculations. Although the OR integral cross section for the 1s-2s excitation is much better than the slowly converging close-coupling results,[8, 51, 80] we might hope that the close-coupling method gives qualitatively correct differential cross sections. The reason is that the validity of the high-energy approximations of first-order methods are often effectively angle-dependent but the close-coupling calculations make no obviously angle-dependent approximation (of course the close-coupling calculations are not equally valid for all partial waves, and thus their predicted angular distributions are not exactly correct). Figures 4–6 compare the 1s-1s exchange differential cross sections at energies of 1.00, 1.44, and 4.00 Ry.[81] Figures 7–10 compare the 1s-2s exchange differential cross sections at energies of 1.00, 1.44, 2.25, and 4.00 Ry. These figures show that in general the BBGM1 and BO angular distributions are in qualitative agreement with the c.c. results.[82] At $(a_0k)^2 = 2.25$ for the 1s-2s exchange collisions, the OR prediction is in serious disagreement with the BSS and BO results from 0 to 35° – this disagreement is the same type as found for small angles in the 2^3S excitation of He as noted above. Figures 9 and 10 for the 1s-2s excitation of the hydrogen atom show that the BSS c.c. results have two peaks. The first-order results omit the peak at 0°. When the first-order results give good values for the integral cross sections they must do this by predicting an increased size for the peak at larger angles. Note that at higher energies the diferential cross sections predicted by all the first-order methods become identical and are all peaked off zero

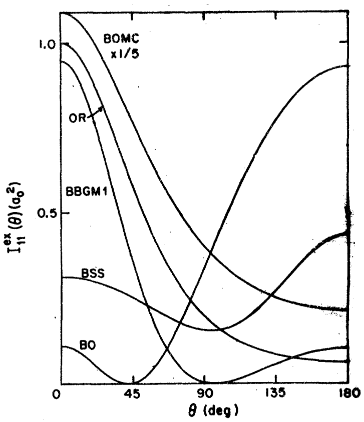

FIG. 4. Differential exchange cross sections (a_0^2) for 1s-1s scattering from the hydrogen atom at $E=1.0$ Ry.

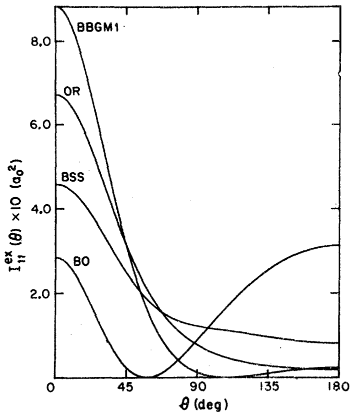

FIG. 5. Differential exchange cross sections (a_0^2) for 1s-1s scattering from the hydrogen atom at $E=1.44$ Ry.

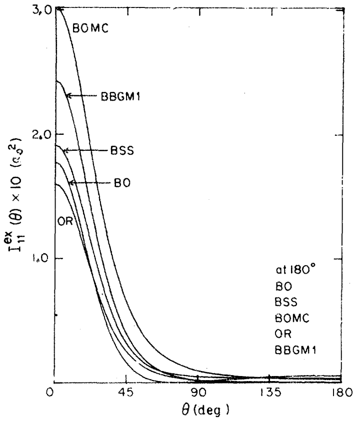

FIG. 6. Differential exchange cross sections (a_0^2) for 1s-1s scattering from the hydrogen atom at $E=4.00$ Ry. The order of the cross sections at 180° is given at right side of the figure.

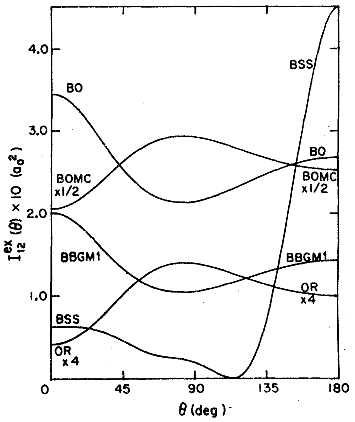

FIG. 7. Differential exchange cross sections (a_0^2) for 1s-2s excitation of the hydrogen atom at $E=1.00$ Ry.

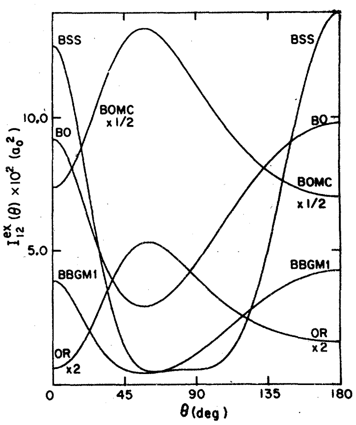

FIG. 8. Differential exchange cross sections (a_0^2) for 1s-2s excitation of the hydrogen atom at $E=1.44$ Ry.

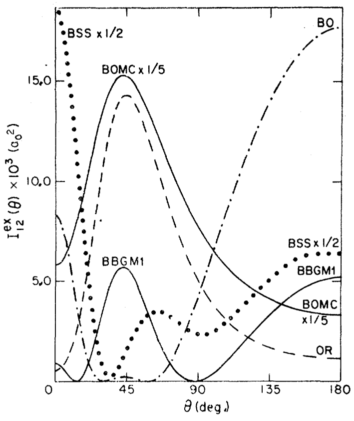

FIG. 9. Differential exchange cross sections (a_0^2) for 1s-2s excitation of the hydrogen atom at $E=2.25$ Ry.

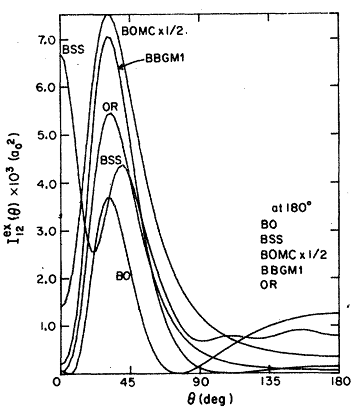

FIG. 10. Differential exchange cross sections (a_0^2) for 1s-2s excitation of the hydrogen atom at $E=4.00$ Ry.

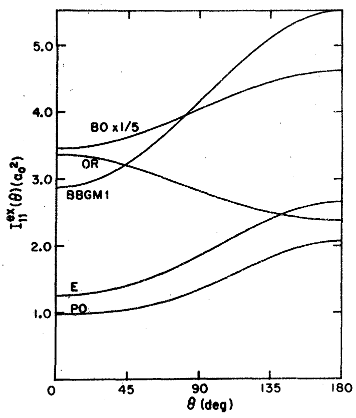

FIG. 11. Differential exchange cross sections (a_0^2) for 1s-1s scattering off the hydrogen atom at $E=0.09$ Ry. Comparison with exchange (E) and polarized orbital (PO) calculations of Ref. 86.

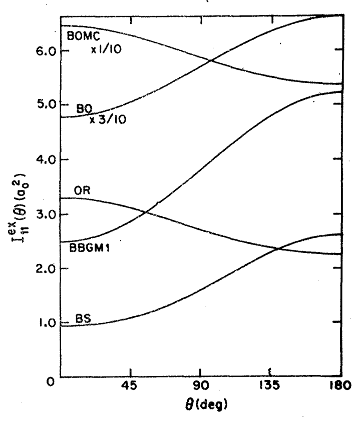

FIG. 12. Differential exchange cross sections (a_0^2) for 1s-1s scattering of the hydrogen atom at $E=0.1$ Ry.

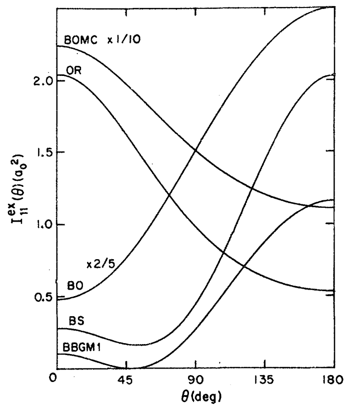

FIG. 13. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 0.4$ Ry.

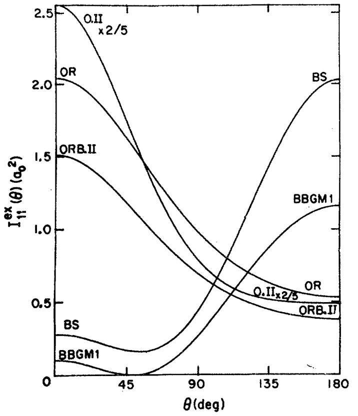

FIG. 14. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 0.4$ Ry.

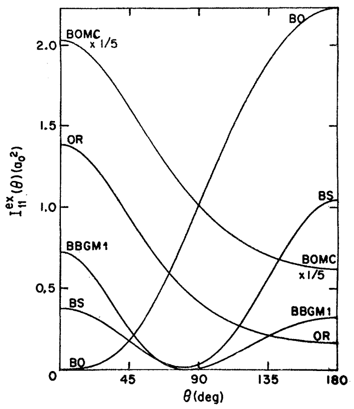

FIG. 15. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 0.7$ Ry.

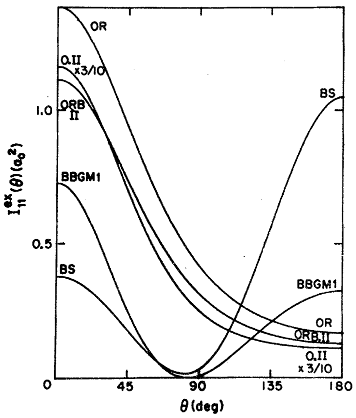

FIG. 18. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 0.7$ Ry. The O.II and ORB. II results are 1 × 1.

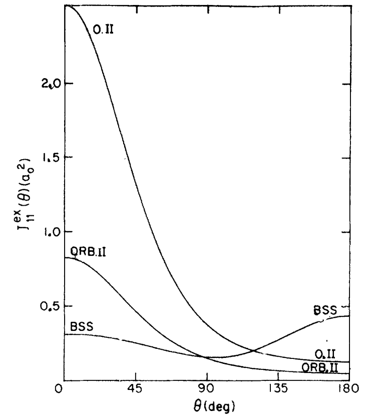

FIG. 19. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 1.0$ Ry. For O.II and ORB. II the 2×2 results are shown. The 1×1 results are higher but the same within 6%.

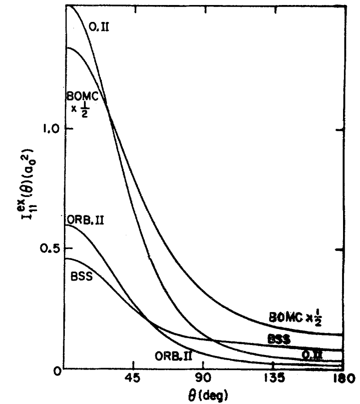

FIG. 20. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 1.44$ Ry. For O. II and ORB. II the 2×2 results are shown. The 1×1 results are higher but the same within 5%.

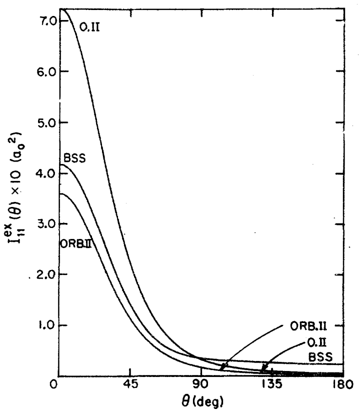

FIG. 21. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 2.25$ Ry. For the O. II and ORB. II calculations, the 2×2 is drawn. The 1 × 1 is the same within 2%, but higher.

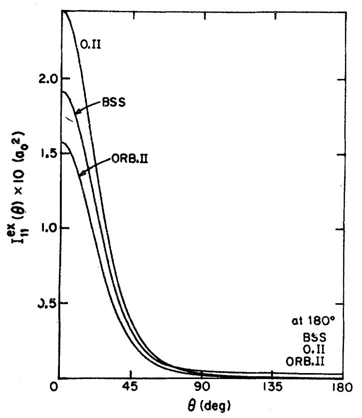

FIG. 22. Differential exchange cross sections (a_0^2) for 1*s*-1*s* scattering off the hydrogen atom at $E = 4.0$ Ry. For the O. II and ORB. II calculations, the 2×2 cases are drawn. The 1×1 calculations are the same within ½%.

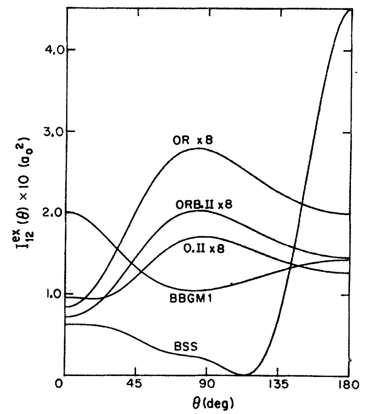

FIG. 23. Differential exchange cross sections (a_0^2) for 1*s*-2*s* excitation of the hydrogen atom at $E = 1.00$ Ry.

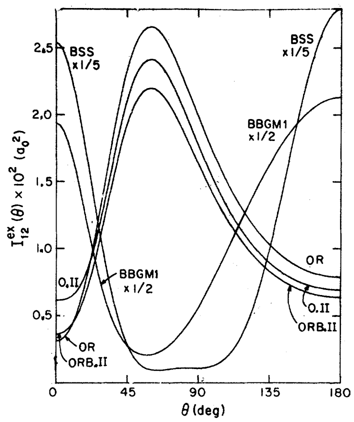

FIG. 24. Differential exchange cross sections (a_0^2) for 1*s*-2*s* excitation of the hydrogen atom at $E = 1.44$ Ry.

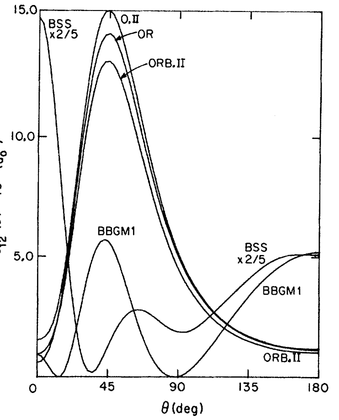

FIG. 25. Differential exchange cross sections (a_0^2) for 1*s*-2*s* excitation of the hydrogen atom at $E = 2.25$ Ry.

degrees. (For the exchange elastic scattering, however, they are all peaked at 0°.) This is illustrated by Table VI which shows the peaks in the differential 1*s*-2*s* exchange cross sections. At high energies the BO approximation predicts the angular distribution rises at large angles to a rather flat section at about 140 to 180°. Even at 1000 eV (where the integral cross sections differ by only 6%) the differential cross sections exhibit marked differences, especially at large angles. This fact is illustrated by the ratios of differential cross sections in Table VII. This table also shows how the cross section is very much shifted toward forward angles at high energies.

3.6 Angular Distribution at Low Energies

The slow convergence of the close-coupling results for intermediate energy scattering off the hydrogen atom does not imply that this approximation is always bad.[80] One important case where the c.c. approximation is expected to be more reliable is in energy ranges where the state expansion includes all open channels.[54] Such a case is the one-state calculation of low-energy elastic scattering. When exchange of identical particles is possible this is called the exchange approximation.[83] In the perturbed stationary state approach[5d] to the exchange approximation, the atom eigenfunction is replaced by an eigenfunction modified by the bound system-incident particle interaction. For electron-atom scattering one way to do this is called the polarized orbital method.[84], [85] Numerical solutions of the exchange (E) and polarized orbital (PO) equations have been carried out by Temkin and Lamkin.[86] We compare elastic exchange differential cross sections from their work at $(a_0k)^2 = 0.09$ with the

TABLE VI. Positions of the peaks in the differential cross section for 1*s*-2*s* exchange excitation off the H atom. Given in degrees is the angle at which differential cross section is greatest among the angles 0(1)12(2)24(6)60(5)180. The notation *A*(x)*B* means from *A* to *B* in steps of x. Highest peaks are listed first and all peaks are listed.

E (eV)	BO	BBGM1	BOMC	OR
12	0, 180	0, 180	100	100
15	0, 180	0, 180	75	75
20	180, 0	180, 0	54	60
25	180, 0	180, 0	48	48
30	180, 0, 42	180, 42, 0	42	48
35	180, 0, 42	42, 180, 0	42	42
40	180, 36, 0	36, 180	36	36
50	30, 180, 0	30, 180	30	36
100	22, 180	22, 180	22	22
150	18, 180	18, 180	18	18
200	16, 180	16	16	16
250	14, 180	14	14	14
300	12, 180	12	12	14
350	12, 180	12	12	12
400	11, 180	11	11	11
500	10, 180	10	10	10
1000	7, 180	7	7	7

TABLE VII. Ratios of values of differential cross sections for 1s-2s exchange scattering. HP = highest peak unless HP would be 180°; then HP is next highest peak. In this table, the number in parentheses is the power of 10 by which the number is to be multiplied.

E (eV)		$\frac{\sigma(180°)}{\sigma(90°)}$	$\frac{\sigma(180°)}{\sigma(\mathrm{HP})}$	$\frac{\sigma(90°)}{\sigma(2°)}$
20	BO	2.24(0)	1.09(0)	4.90(-1)
	BBGM1	4.09(0)	1.15(0)	2.82(-1)
	OR	3.83(-1)	2.80(-1)	6.43(0)
40	BO	5.82(0)	2.02(0)	7.45(-1)
	BBGM1	1.29(1)	1.35(-1)	4.24(0)
	OR	1.71(-1)	3.28(-2)	7.27(0)
100	BO	9.89(0)	2.86(-2)	3.07(-1)
	BBGM1	5.42(-2)	3.61(-2)	1.47(-1)
	OR	9.65(-2)	1.22(-1)	1.83(0)
400	BO	7.10(0)	1.84(-4)	1.14(-3)
	BBGM1	4.40(-2)	4.90(-6)	4.14(-3)
	OR	6.70(-2)	5.74(-6)	6.26(-3)
1000	BO	5.35(0)	5.80(-6)	1.63(-5)
	BBGM1	6.89(-2)	2.36(-7)	5.05(-5)
	OR	6.54(-2)	1.52(-7)	3.96(-5)

BO, BBGM1, and OR results in Fig. 11. The good agreement of the E and PO angular distribution is consistent with our expectation of their reliability. The BBGM1 and BO methods again appear to predict reliable angular distributions. The OR method shows the opposite trend. Another calculation by Temkin and Lamkin,[86] the exchange-adiabatic approximation[85] (not shown), also predicted a cross section decreasing monotonically from 0°, as the OR does. Figures 12-15 compare the first-order calculations of the exchange elastic process with 1s-2s-2p c.c. calculations of Burke and Schey.[43] These c.c. calculations should be even more accurate than the exchange approximation. They agree with experiment[87] on the total differential cross section at energies 3.8-9.4 eV.[43] Again the shapes of the BBGM1 and BO differential cross sections are in better agreement with BSS one than the OR and BOMC results.

3.7 Unitarization and the ORB. II Results

According to Eq. (31) the lth partial-wave cross section is given by

$$\sigma_l^{\text{ex}} = (\pi/k^2)(2l+1)|T^{l,\,\text{ex}}|^2 . \qquad (38)$$

The requirement that the flux of scattered particles in a particular partial wave cannot exceed the total flux present in that partial wave then requires[3b]

$$|T_{\text{elas}}^{\ l}| \leq 2, \qquad (39)$$

$$|T_{\text{inelas}}^{\ l}| \leq 1.$$

The third and fourth columns of Table VIII show some typical $\underline{T}$ elements in the O and OR approximations. As seen, the O approximation violates the conservation theorem near zero energy for both elastic processes, but the OR calculations do not ever exceed these limits. Table VIII also shows unitarized calculations obtained by truncating the R matrix to 1×1 and 2×2 before using Eq. (18). These $\underline{T}$ elements automatically satisfy the limits (39). Starting with an $N\times N$ R matrix insures that, in any partial wave, the sum of particles scattered both elastically (in any channel) and by any of the $N-1$ inelastic processes initiating in that channel does not exceed the total flux of particles present in that partial wave. The 1×1 case is often called allowance for back coupling and the $N\times N$ case ($N>1$) is often called allowance for strong coupling. Also shown in Table VIII are $\underline{T}$ elements obtained from the phase shifts of Burke and Schey[43] and the 4×4 R matrix of Burke, Schey, and Smith.[44] These also automatically satisfy the limits (39).

Table VIII compares typical $\underline{T}$ elements before (I) and after (II) unitarization. The comparison shows that the unitarization procedure makes the biggest difference when one of the partial cross sections involved exceeds the conservation limits. Figure 16 shows integral elastic exchange cross sections calculated in the close coupling and unitarized first-order approximations (above threshold we show the 2×2 results for O. II and ORB. II although the 1×1 results are very close to these). This figure shows that the ORB. II cross sections are quite good. Figure 17 shows the integral 1s → 2s exchange cross sections calculated in the unitarized approximations and obtained from experiment. It is interesting that near threshold the O. II 1s → 2s cross section is less than the ORB. II curve. This is because the O approximation pre-

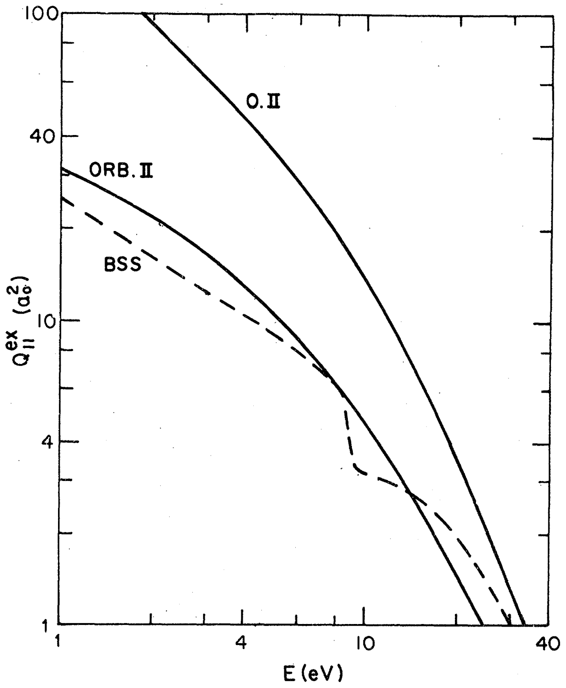

FIG. 16. Integral exchange elastic scattering cross sections for the hydrogen atom.

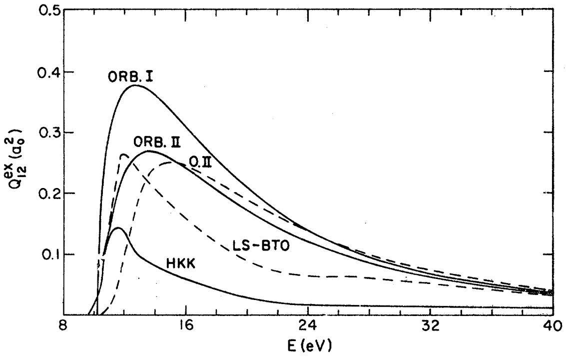

FIG. 17. Integral 1*s*-2*s* exchange excitation cross sections for the hydrogen atom.

dicts much too large cross sections for the $2s \rightarrow 2s$ scattering in this region. When the $1s \leftrightarrow 2s$ and $2s \leftrightarrow 2s$ processes are coupled together, the $2s \rightarrow 2s$ then "steals" most of the transition probability. Such drastic effects do not occur in the correctly normalized ORB. II method. The ORB. II result agrees with experiment near threshold.

Figures 18-25 show differential cross sections calculated in the unitarized approximation. As seen by comparison with Figs. 4-9, the shape of the angular distribution is not much affected by the procedure for either the elastic or inelastic processes. Thus the ORB. II angular distribution, like the OR angular distribution, retains its high-energy form down to low energies and becomes in error there as the experimental angular distribution necessarily becomes more isotropic.

4. FURTHER DISCUSSION

4.1 Basic Limitation of the Born Approximation at Intermediate Energies

The special difficulties of the BO approximation for rearrangements (not shared by the Born approximation for direct scattering) appear to be associated with core and orthogonality problems. The BBGM1 approximation and the *E*1 approximation correct these features. But a difficulty still remains; neglect of polarization in the atom and distortion in the scattered wave makes an important difference at the low and intermediate energies where contributions from rearrangement are appreciable. The nominal criterion for the validity of the Born approximation for electronic re-

TABLE VIII. $\left| T^{l,\mathrm{ex}} \right|$.

	E (Ry)	*l*	O. I	OR	O. II 1×1	ORB. II 1×1	O. II 2×2	ORB. II 2×2	BSS 4×4	BSS 2×2
1*s*-1*s*	0.1	0	11.4992	1.0454	1.9704	0.9265			0.7966	
		1	0.3652	0.0332	0.3593	0.0332			0.0983	
	0.4	0	4.5175	1.2907	1.8288	1.0845			0.8319	
		1	0.5048	0.1442	0.4894	0.1438			0.3634	
		2	0.0508	0.0145	0.0508	0.0145			0.0034	
	0.7	0	2.8123	1.1580	1.6299	1.0021			0.3382	
		1	0.4928	0.2029	0.4785	0.2019			0.4489	
	1.0	0	2.0000	1.0000	1.4142	0.8944	1.3764	0.8668	0.6241	0.8998
		1	0.4548	0.2274	0.4435	0.2260	0.4435	0.2259	0.4069	0.4155
	4.0	0	0.4000	0.3200	0.3922	0.3160	0.3906	0.3148	0.2892	0.2818
		1	0.1976	0.1581	0.1967	0.1576	0.1966	0.1575	0.2188	0.2140
1*s*-2*s*	0.7718	0	0.2931	0.2214			0.0177	0.1495		
		1	0.0075	0.0057			0.0051	0.0056		
	1.0	0	0.4267	0.3413			0.2673	0.2906	0.2725	0.0399
		1	0.0090	0.0072			0.0081	0.0070	0.0767	0.1857
		2	0.0177	0.0141			0.0172	0.0140	0.1525	0.1348
		3	0.0056	0.0050			0.0056	0.0045	0.0426	0.0175
	2.25	0	0.2423	0.2181			0.2209	0.2071	0.1331	0.2062
		1	0.0471	0.0424			0.0465	0.0421	0.0865	0.1993
	4.0	0	0.1239	0.1166			0.1210	0.1147	0.0885	0.0990
		1	0.0455	0.0428			0.0453	0.0427	0.0679	0.0592
		2	0.0091	0.0086			0.0091	0.0086	0.0095	0.0103
2*s*-2*s*	0.0218	0	20.2606	1.6233	1.9903	1.2604	1.9902	1.2485		
		1	2.0667	0.1656	1.4372	0.1650	1.4372	0.1650		
	0.25	0	1.0000	0.5000	0.8944	0.4851	0.8467	0.4559	0.5762	0.9939
		1	0.8193	0.4096	0.7581	0.4013	0.7581	0.4013	0.5285	0.8009
	1.50	0	0.1523	0.1306	0.1519	0.1303	0.1421	0.1247	0.1619	0.1636
		1	0.0524	0.0449	0.0524	0.0449	0.0522	0.0448	0.1088	0.2000
	3.25	0	0.0639	0.0593	0.0638	0.0593	0.0626	0.0584	0.0604	0.0557
		1	0.0274	0.0255	0.0274	0.0255	0.0273	0.0254	0.0420	0.0339

arrangement is that the initial relative velocity must exceed the orbital velocity of the electron.[88] For reaction (1) this implies an energy much greater than 13.6 eV and for process (36) an energy much greater than 25 keV. The region below these velocities is called the low-energy region.[88] The errors in the Born approximation for direct scattering in the low and intermediate energy regions provide a reasonable limit for what improvement one can expect by eliminating the special rearrangement difficulties. Note that in the higher energy region where the Born approximation for direct scattering is truly valid, the exchange scattering is negligible or very small.

The error that may be inherent in the first-order treatment is shown by Tables IX and X. Table IX compares approximations to the R matrix, and Table X compares the same results after unitarization on a four-state basis ($1s$, $2s$, $2p_{-1}$, and $2p_{+1}$). Part A of Table IX is adapted from Lawson, Lawson, and Seaton.[89] Part A of Table X is from Burke and Seaton.[37] These Born-approximation results are compared with results of the close-coupling calculations of Burke, Schey, and Smith.[44] As evident from these tables, the accuracy of the Born approximation (relative to the BSS c.c. results) improves as the relative kinetic energy and angular momentum of the incident particle increases. These calculations also illustrate the effect of unitarization and show again that this is less important when the cross sections are smaller.

TABLE IX. Direct scattering. $|T^{\mathrm{I}}| = 2|R|$: (A) from Born direct calculation of Lawson, Lawson, and Seaton (1961) and (B) from BSS three-state c.c. calculations.

E (Ry)	l	$1s$–$1s$	$1s$–$2s$	$2s$–$2s$
		A		
1.0	0	1.1932	0.4424	5.1361
	1	0.1932	0.1264	1.6362
	2	0.0342	0.0292	0.5008
	3	0.0062	0.0060	0.1406
2.25	0	1.2474	0.3634	3.5170
	1	0.3242	0.2226	1.9602
	2	0.0938	0.1158	1.2210
	3	0.0278	0.0550	0.7674
4.00	0	1.2048	0.2790	2.8120
	1	0.4048	0.2118	1.7346
	2	0.1530	0.1420	1.2164
	3	0.0596	0.0884	0.8832
		B		
1.0	0	7.4945	4.5473	16.7994
	1	0.5544	0.9376	5.2885
	2	0.2142	0.0369	1.4345
	3	0.0730	0.0168	0.4722
2.25	0	1.7483	2.0067	6.2011
	1	0.4571	0.6159	2.5863
	2	0.1738	0.1432	1.5806
	3	0.0754	0.0488	0.9750
4.00	0	2.0585	2.0716	12.7441
	1	0.5038	0.3689	2.5853
	2	0.1875	0.1851	1.4547
	3	0.0798	0.0993	1.0047
	6	0.0158	0.0108	0.3845

In an effort to improve the Born approximation, Rudge has proposed[8] an extension of the OR method to calculate direct scattering. This result was subsequently modified by Morrison and Rudge[15] (MR) to insure compatibility of the phases for direct and exchange (OR) amplitudes. Table XI compares the Born direct and BO exchange approximations with the MR results for direct and exchange integral cross sections. In accordance with the discussion of the previous paragraph, the corresponding differences are much larger for the exchange case than for the direct case. The MR results show a substantial improvement over the Born results. This subtle MR correction to the Born approximation for direct scattering deserves further study and could be of great usefulness if it generally provides improvement.

4.2 Improvements over the First-Order Model

The methods discussed in Secs. 2.1 to 4.1 are derived from first-order approximations in which the transition is calculated between two undistorted wave functions for the incident and scattered electrons and unpolarized basis sets for the bound electrons but the interaction potential is refined. One possible improvement is to modify these wave functions by the core interaction (here $1/r_2$), the rearrangement term in the interaction (here $1/r_{12}$) or both. One method for doing this, the perturbed stationary state approach, was already discussed in Sec. 3.6. In this perturbed stationary state approach, the bound-state wave functions are modified by the interaction with the incident particle and the scattering is calculated with these adiabatically perturbed states. In another method, the distorted-wave approximation [also called the distorted-wave Born approximation (DWBA)], the incident particle wave function is modified by its interaction with the bound system. One way in which the DWBA can be applied to electron-atom scattering is in the form of the Coulomb wave approximation (CWA) in which the incident-particle wave function is modified by the (unscreened) core of the bound system and not by the rearrangement term. For electron-atom collisions, this often leads to worse results than the use of undistorted waves.[1b] Such a result is expected for general rearrangements whenever the screened core (entire initial bound system) is a much smaller perturbation of the incident particle's motion than the unscreened core. In this case the exact scattering waves resemble plane waves more than they resemble core-distorted waves. Oppenheimer himself[2] pointed out this difficulty of the CWA for process (1). Beigman and Vainshtein[10] have calculated the $1s-2s$ excitation cross section for $e^- - H$ scattering in the CWA. They found the result was better than the BO approximation but worse than the O approximation in the energy range 10.24 to 35 eV. They also point out that the CWA predicts a large cross section at the excitation threshold (in the $1s-2s$ case it gives a total integral cross section of $1.5a_0^2$ at threshold[10]). Further, since the scattering waves are not plane waves, the calculations are more difficult than the first-order methods considered here. The CWA does, however, have

TABLE X. Direct scattering. $|T^{\mathrm{II.}\ 4\times 4}|$: (A) from Burke-Seaton Born II Calculation and (B) from BSS three-state c.c. calculation.

E (Ry)	l	1s-1s	1s-2s	2s-2s
		A		
1.0	0	1.0008	0.1257	1.7818
	1	0.1597	0.0406	1.1318
	2	0.0326	0.0750	0.8309
	3	0.0093	0.0485	0.7407
2.25	0	1.0310	0.1540	1.7213
	1	0.2920	0.1501	1.3706
	2	0.0736	0.0795	0.9873
	3	0.0337	0.0484	0.6600
4.00	0	1.0127	0.1391	1.6177
	1	0.3769	0.1543	1.2963
	2	0.1368	0.1135	1.0222
	3	0.0518	0.0719	0.7834
		B		
1.0	0	1.4405	0.2852	0.9239
	1	0.8822	0.1763	0.8905
	2	0.1837	0.1116	1.1049
	3	0.0622	0.0558	0.7166
2.25	0	1.2600	0.2106	1.5766
	1	0.3836	0.2359	1.5681
	2	0.1187	0.0923	1.2202
	3	0.0658	0.0511	0.8287
4.00	0	1.2002	0.1995	1.8096
	1	0.4361	0.2230	1.5065
	2	0.1607	0.1419	1.1645
	3	0.0669	0.0781	0.8822

some formal advantages such as orthogonality of initial and final states and automatic satisfaction of the conservation theorems.[11]

For electron-atom collisions, the recent approximation of Vainshtein, Presnyakov, and Sobel'man[90, 91, 32] puts the effect of the rearrangement term $1/r_{12}$ into the relative motion wave function itself. However, the applications of this method have involved computational approximations of uncertain validity and the method has not been tested sufficiently to ascertain its usefulness.

4.3 Improved First-Order Methods

Another improved method for electron exchange collisions has been proposed by Beigman and Vainshtein.[10] In it, the initial and final particle wave functions are approximated using plane-wave scattering functions and then orthogonalized to the corresponding final- and initial bound-state particle wave functions, respectively. This method appears to give reasonably accurate integral exchange cross sections for electron-atom collisions[10] and deserves further study. It is not difficult to apply if the approximate bound state wave functions are Hartree wave functions, i.e., not antisymmetrized.

All the modified BO methods discussed above are essentially first order in that they assume the BO or BBGM1 approximation is correct or nearly correct at large energy. However, this assumption may be erroneous. Recent calculations on process (36) have shown that second-order methods often differ significantly at high energy from these first-order treatments.[92–94]. Further, the whole structure of these approximate treatments is questioned by the possible divergence of the Born[95] and distorted-wave Born[96] series for rearrangement collisions. Another possibility is that the Born series converges but not to its first term, even at high energy.[94] Dodd and Greider[97] point out that the usual approximations (such as BO and DWBA) are "intuitive models based primarily on semiclassical concepts of direct reactions" and that such models may be inadequate for rearrangements. This inadequacy and the divergences mentioned above are due to the pathological nature of the kernel of the nonhomogeneous Lippmann-Schwinger integral equation for rearrangements when the Born term or distorted-wave Born term is used as the nonhomogeneous term.[98] In principle, these difficulties might be avoided by using the Fadeev equations.[99] Dodd and Greider[97] developed a consistent first-order approximation to the Fadeev equations and found their results were similar to the results of the variational calculations for rearrangements of Lippmann[100] and Joachain.[93] The Fadeev-Dodd-Greider method and the Joachain variational method do not begin by assuming that either the BO approximation or the DWBA is correct or nearly correct at any energy. Such an assumption is, however, contained in the ORB.II, BBGM1, and other first-order results discussed above. Further theoretical work will be necessary to resolve these inconsistencies. Calculations by the Fadeev-Dodd-Greider first-order method (FDG1) are appreciably harder than the first-order calculations reported here. McCarroll and Salin[101] made an investigation of process (36) by the FDG1 method and concluded that Q^{FDG1} tends to the second Born-approximation value at high energies. However, their analysis is not rigorous[102] and, as a result, the problem of the exact high-energy limit remains unresolved.[102,94]

TABLE XI. 1s-2s integral cross sections (a_0^2). In this table, the number in parentheses is the power of 10 by which the number is to be multiplied. The MR results are from Ref. 15.

E (Ry)	$Q_{12}{}^d$	$Q_{12}{}^d$	$Q_{12}{}^d$	$Q_{12}{}^{\mathrm{ex}}$
	Born	MR	BO	OR
0.76	2.49(-1)	1.12(-1)	2.17(0)	1.40(-1)
0.80	5.09(-1)	2.38(-1)	3.88(0)	2.81(-1)
0.90	7.21(-1)	3.64(-1)	3.91(0)	3.73(-1)
1.00	7.80(-1)	4.21(-1)	3.02(0)	3.70(-1)
1.30	7.53(-1)	4.68(-1)	1.11(0)	2.64(-1)
2.00	5.75(-1)	4.21(-1)	1.36(-1)	1.03(-1)
3.00	4.13(-1)	3.36(-1)	2.46(-2)	3.56(-2)
4.00	3.20(-1)	2.74(-1)	1.14(-2)	1.60(-2)
20.00	6.86(-2)	6.66(-2)	1.59(-4)	1.43(-4)
50.00	2.77(-2)	2.74(-2)	9.97(-6)	9.32(-6)
Born II for direct				
1.00	2.23(-1)			
4.00	2.32(-1)			

TABLE XII. Rearrangement collision amplitudes.

	BO	BOMC	BBGM1	O	O.II	OR	ORB.I	ORB.II	CWA	BV	c.c.
Includes core	Yes	No	No	No[12]	No	No	No	No	No	No	...
Orthogonal waves	No[2]	No	Effectively[7]	Yes[23]	Yes	Yes[8,23]	Yes[23]	Yes	Yes[11]	Yes[10]	Yes[106]
Variational principle	Yes[3(h)]	No[3(e)]	No[3(e),105]	No[8]	No	Yes[8,23]	Yes[23]	Yes[23]	...	...	Yes[107]
Post-prior discrepancy	Yes[3(d)]	No	Yes	Yes[12]	No	Yes[64]	No	No	No	No	No
Detailed balance	Yes	Yes	Yes	Yes[23]	Yes	No[16,23,64]	Yes[23]	Yes	Yes	Yes	Yes
Conserves flux	No[1(c),11]	No	No	No	Yes	No	No	Yes[3(f)]	Yes[11]	No	Yes

Note added in proof: McDowell pointed out the significant new work done by Dettman and Leibfried, Z. Physik 210, 43 (1968). They show that, for a linear model of process (35) with quite general potentials, the Born rearrangement series converges at high energy to the second Born approximation with cross section $\frac{4}{9}\,Q^{\mathrm{BK}}$. See also Corbett, J. Math. Phys. 9, 891 (1968) for a reconciliation of the two articles in footnote 95.

5. SUMMARY

Several approximations for rearrangement collisions have been applied to the electron exchange scattering off the H atom. It is found that the BO amplitude is dominated by the core term at low energies but correction for this defect is not simple. A delicate balance of forces dictates the scattering, and, hence, if allowance for distortion is introduced it must be done consistently. The ORB.II method predicts excellently the shape and height at maximum of the exchange excitation integral cross section curve versus energy and also predicts very well the exchange elastic scattering. The BBGM1 method and the c.c. method give similar angular distributions for elastic and inelastic processes. However, the BBGM1 method predicts integral cross sections poorly at low energy and, if the c.c. results are taken as accurate, the OR and ORB. II methods predict angular distributions poorly. The OR and BOMC methods predict similar angular distributions for the excitation process, rising with angle at small angles where the differential cross sections predicted by the BO and c.c. methods are falling.

TABLE XIII. Glossary of abbreviations.

BBGM1	Bates, Bassel, Gerjuoy, and Mittleman first-order method
BO	Born-Oppenheimer approximation
BOMC	BO approximation without the core term
BV	Method of Beigman and Vainshtein
c.c.	Close coupling method
CWA	Coulomb wave approximation
DWBA	Distorted wave approximation
E1	First-order exchange method
MR	Method of Morrison and Rudge
O	Ochkur method
O.II	Unitarized Ochkur approximation
OR	Ochkur-Rudge method
ORB.I	Ochkur-Rudge-Bely method I
ORB.II	Unitarized Ochkur-Rudge-Bely approximation
PO	Polarized orbital method

6. ADDENDUM

After the present paper was completed, a letter by Rudge[103] was published in which he argued on theoretical grounds against the Day, Sucher, and Kang, *et al.*[4] suggestion of always dropping the core term from the BO amplitude. Our results show numerically that the core term should not be dropped from the BO amplitude (except possibly at high energies if it is small there). Together with Rudge's analysis, our results thus offer a convincing argument against the BOMC approximation for electron-atom scattering.

APPENDIX

Table XII summarizes some of the properties of approximate methods discussed in this paper and gives some references where further comments may be found. The table answers these questions: (1) Does the approximate scattering amplitude contain a contribution from the matrix element of the core term? (2) Are the initial and final system wave functions orthogonal? (3) Can the method be derived from a variational pricicple? The answers to this question depend somewhat on the point of view adopted and how the class of admissable functions is limited. We have not used a consistent approach in answering this question. The most significant point is that the Ochkur amplitude can be derived from an improperly normalized function.[104] (4) Is there a discrepancy between post and prior formulations if approximate bound-state wave functions are used? (5) Do the results satisfy detailed balance for exact bound-state wave functions and a proper choice among post and prior forms for each direction of reaction? (6) Does the method conserve particle flux automatically?

Table XIII is a glossary of abbreviations used in Table XII and elsewhere in the text.

Discussions of other aspects of rearrangement collisions may be found in recent reviews by Bransden,[108] Peterkop and Veldre,[109] and Moiseiwitsch and Smith.[110]

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*This work was supported by the U.S. Atomic Energy Commission, Report Code: CALT-532-28.

†Work performed in partial fulfillment of the requirements for the Ph. D. degree in chemistry from the California Institute of Technology.

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§Contribution No. 3665.

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[81] 1 Ry = 0.5 hartree = 13.605 eV. Thus the energy $E = (\hbar k)^2/2m$ is 1 Ry when $(a_0k)^2 = 1.0$. In this paper we use both Ry and eV to facilitate comparison with other work.

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electrons from He at 75–350 eV calculated in the first and second Born approximation. At these energies they find the first-order method's predicted relative peak at 0° is too small in comparison with either the second Born approximation or the experimental results.

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