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Effect of Second-Order Exchange in Electron-Hydrogen Scattering

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The electron-hydrogen scattering problem has been a nemesis to theoretical atomic physicists due to the fact that even the most sophisticated of theoretical calculations, both perturbative and nonperturbative, do not agree with experiment. The current opinion is that the perturbative approach cannot be used for this problem since recent second-order calculations are not in agreement with the experimental data and higher-order calculations are deemed impractical. However, these second-order calculations neglected second-order exchange. We have now added exchange to the second-order calculation and have found that the primary source of disagreement between experiment and theory for intermediate energies is attributable not to higher-order terms but to second-order exchange.

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Electron-hydrogen scattering is one of the fundamental problems of atomic physics and has been studied numerous times both theoretically and experimentally. One of the intriguing aspects of this problem is that agreement between experiment and even the most sophisticated of current theories is not satisfactory. If one wishes to examine this problem theoretically, there are two approaches which may be used—the close-coupling approach or the perturbation-series approach. The primary advantage of the perturbation-series approach is that different physical effects can be isolated and examined. A review of the perturbation-series method was given by Walters.¹ If one compares first-order perturbation-series results with experiment, qualitative agreement is found, but the agreement is not satisfactory. The immediate conclusion is that second-order or perhaps higher-order terms are important. Some early second-order calculations were performed¹ which seemed to improve agreement between experiment and theory, but again the agreement was not satisfactory. These early calculations, however, invoked several simplifying approximations in the evaluation of the second-order amplitude so it was felt that the problem might lie in the approximations producing a poor representation of the second-order amplitude. These works were followed by some second-order calculations which did not make simplifying approximations—a second-order plane-wave Born calculation for $2s$ excitation of hydrogen by Ermolaev and Walters² and some extensive second-order distorted-wave calculations by our group for excitation of both the $2s$ and $2p$ states^{3,4} of hydrogen. Again these second-order results were not in satisfactory agreement

with experiment for scattering from the most elementary atom hydrogen.

These latter calculations included first-order direct and exchange terms and second-order direct-scattering terms. Initially it was not expected that second-order exchange would be important since first-order exchange was fairly small, particularly at intermediate energies. However, close-coupling results indicated that second-order exchange may be important so we decided to examine its effect. In this paper, we report the first results of an exact calculation of the effects of second-order exchange, where we define “exact” to mean that no approximations are made in the evaluation of the amplitude. We have found that not only is second-order exchange important, most importantly it brings theory and experiment into very good agreement for both elastic scattering and inelastic scattering for quantities which depend on the magnitude of the amplitude. As will be demonstrated, second-order exchange transforms state-of-the-art perturbation-series results which are mediocre and disappointing into results which agree with experimental differential cross sections and λ parameters⁵ as well as one could reasonably hope for.

The exact T matrix for electron-hydrogen scattering with complete allowance for exchange is given by Eq. (161) of Goldberger and Watson.⁶ This result was obtained for the case of the incoming and outgoing projectiles being represented by a plane wave. If one expresses the initial- and final-state plane waves in terms of initial- and final-state distorted waves, it can be shown that the exact T matrix in the distorted-wave representation is given by

$$T_{fi} = 2\langle\chi_f^-(0)\psi_f(1)|V-U_f|A\psi_i(1)\chi_i^+(0)\rangle + \langle\chi_f^-(0)\psi_f(1)|U_f|\psi_i(1)\beta_i(0)\rangle \\ + 2\langle\chi_f^-(0)\psi_f(1)|(V-U_f)A(E^+ - H)^{-1}A(V-U_i)|\psi_i(1)\chi_i^+(0)\rangle, \quad (1)$$

where ψ_i and ψ_f are the initial and final atomic wave functions and H is the Hamiltonian for the system,

$$H = h_a + T_0 + V, \quad (2)$$

where h_a is the Hamiltonian for the hydrogen atom, T_0 is the kinetic-energy operator for the projectile, and V is the interaction between the projectile and the atom (nuclear interaction plus electron-electron interaction). The distorting potentials U_i and U_f are initial- and final-state spherically symmetric approximations for V and these potentials are used to calculate the distorted waves χ_i and χ_f ,

$$(T_0 + U_m - K_m^2)\chi_m = 0, \quad (3)$$

where $m = i$ or f and K_m^2 is the corresponding energy of the projectile electron. The remaining undefined quanti-

ties are β_i which is an initial-state plane wave, $(E^+ - H)^{-1}$ which is the full Green's function for the scattering problem, and A which is the antisymmetrizing operator

$$A = \frac{1}{2} [1 + (-1)^s P_{01}], \quad (4)$$

where P_{01} is the operator which interchanges particles 0 and 1 and where $s=0$ corresponds to singlet scattering and $s=1$ corresponds to triplet scattering.

The factor which prohibits the exact evaluation of Eq. (1) is the full Green's function $(E^+ - H)^{-1}$. Standard perturbation-series expansions result from (1) when a series expansion is made for the Green's function:

$$(E^+ - h_a - T_0 - V)^{-1} = (E^+ - h_a - T_0 - U)^{-1} + (E^+ - h_a - T_0 - U)^{-1}(V - U)(E^+ - h_a - T_0 - U)^{-1} + \dots, \quad (5)$$

where U is a third distorting potential. For the standard development of perturbation series^{1,7} U is set to zero and Eq. (5) is the expansion of the full Green's function in terms of the free-particle Green's function. If U is non-zero, (5) represents the expansion of the full Green's function in terms of a distorted Green's function, and we have allowed for this possibility since one would logically assume that the distorted-Green's-function series would converge more rapidly. The second-order perturbation series is obtained by truncating the expansion (5) after the first term. With this truncation, the second-order amplitude becomes

$$\begin{aligned} T_{fi} = & \langle \chi_f^-(0) \psi_f(1) | V_f(0,1) | \psi_i(1) \chi_i^+(0) \rangle + \langle \chi_f^-(0) \psi_f(1) | U_f(0) | \psi_i(1) \beta_i(0) \rangle \\ & + (-1)^s \langle \chi_f(0) \psi_f(1) | V_f(0,1) | \psi_i(0) \chi_i^+(1) \rangle \\ & + \frac{1}{2} \sum_N \langle \chi_f^-(0') \psi_f(1') | V_f(0',1') | \phi_N(1') g_N^+(0',0) \phi_N^*(1) | V_i(0,1) | \psi_i(1) \chi_i^+(0) \rangle \\ & + \frac{1}{2} (-1)^s \sum_N \langle \chi_f^-(1') \psi_f(0') | V_f(1',0') | \phi_N(1') g_N^+(0',0) \phi_N^*(1) | V_i(0,1) | \psi_i(1) \chi_i^+(0) \rangle \\ & + \frac{1}{2} (-1)^s \sum_N \langle \chi_f^-(0') \psi_f(1') | V_f(0',1') | \phi_N(1') g_N^+(0',0) \phi_N^*(1) | V_i(1,0) | \psi_i(0) \chi_i^+(1) \rangle \\ & + \frac{1}{2} \sum_N \langle \chi_f^-(1') \psi_f(0') | V_f(1',0') | \phi_N(1') g_N^+(0',0) \phi_N^*(1) | V_i(1,0) | \psi_i(0) \chi_i^+(1) \rangle, \end{aligned} \quad (6)$$

where

$$V_f(j,k) = -\frac{2z}{r_j} - U_f(r_j) + \frac{2}{r_{jK}} \quad (7)$$

and

$$V_i(j,k) = -\frac{2z}{r_j} - U_i(r_j) + \frac{2}{r_{jK}}. \quad (8)$$

In Eq. (6), ϕ_N is the intermediate atomic state (discrete or continuum) and the sum implies a sum over discrete and an integral over continuum intermediate states. This sum and integral was performed numerically until convergence was achieved, similar to the calculation of Madison and Winters.³ Finally, the distorted Green's function is given by

$$g_N^+(0',0) = \langle r_{0'} | [E^+ - \epsilon_N - T_0 - U]^{-1} | r_0 \rangle, \quad (9)$$

where ϵ_N is the energy of the intermediate state ϕ_N .

The various terms of Eq. (6) can be identified as follows: first term—first-order direct-scattering amplitude for inelastic scattering; second term—first-order direct-scattering amplitude for elastic scattering; third term—first-order exchange amplitude; fourth term—second-

order direct-scattering amplitude; fifth term—second-order exchange amplitude for which the atomic electron goes to the intermediate atomic and then to the final projectile state; sixth term—second-order exchange amplitude for which the atomic electron goes to the intermediate projectile state and then the final projectile state; and seventh term—second-order exchange amplitude for which the atomic electron goes into the intermediate projectile state and then back into the final atomic state. In our previous works,^{3,4} the first four terms were evaluated but not the last three second-order exchange terms. The last exchange term might reasonably be called a direct process since the atomic electron is finally in the atom and the projectile electron is in the detector, but we classify it as an exchange process since it results from the exchange operator and does not arise without it.

We have calculated second-order amplitudes including these three exchange terms exactly. Obviously, this is a significantly more difficult calculation since there are now four independent second-order amplitudes which need to be evaluated. Our results for the differential cross section for elastic scattering, $2s$ excitation, and $2p$

excitation of hydrogen are shown in Fig. 1. For each case, three results are shown: (1) first-order results which we label DWB1; (2) second-order direct-scattering-only results for the case of $U=0$ which we label DWB2D(g_0); and (3) second-order results including second-order exchange for the case of $U=U_{1s}$, where U_{1s} is the distorting potential for the ground state of hydrogen [we label this calculation DWB2E(g_{1s})]. The selection $U=U_{1s}$ was made since this choice gives somewhat better agreement with experimental data than $U=0$ as will be noted later. From Fig. 1 it is seen that the second-order direct term generally tends to improve agreement with experiment but that the agreement is certainly not as good as is desirable. However, when second-order exchange is added, agreement between experiment and theory becomes very good. We also calculated second-order-exchange results for the case of $U=0$ which we would label DWB2E(g_0). The DWB2E(g_0) results and the DWB2E(g_{1s}) results for the differential cross section would be very similar in a journal figure.

Angular correlation parameters are an even more sensitive test of theory than differential cross sections. In Fig. 2 our results are compared with experiment for the λ and R parameters.¹¹ For these parameters, the DWB2E(g_{1s}) results are in good agreement with experi-

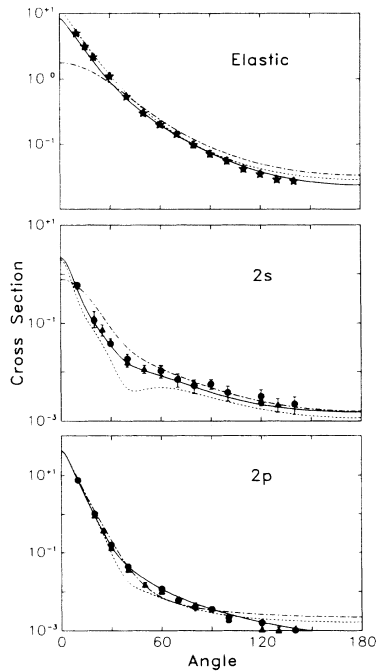


FIG. 1. Differential cross section in units of a_0^2 for elastic and inelastic electron-impact excitation of hydrogen. The incident electron energy is 50 eV for elastic scattering and 54.4 eV for inelastic scattering. The experimental data are from (★) Williams (Ref. 8); (▲) Frost and Weigold (Ref. 9); and (●) Williams (Ref. 10). The theoretical curves are (dash-dotted line) DWB1; (dotted line) DWB2D(g_0); and (solid line) DWB2E(g_{1s}).

ment over the entire angular range for the λ parameter and for angles out to 60° for the R parameter. The large-angle R parameter represents the only case where we found a significant disagreement between experiment and the DWB2E(g_{1s}) calculations. Distortion in the Green's function is more important for the λ and R parameters than it was for the differential cross section. For the case of the λ parameter, DWB2E(g_{1s}) has a higher maximum near 50° and a deeper minimum near 100° than does DWB2E(g_0). Since the primary improvement was due to second-order exchange, the DWB2E(g_0) results are omitted for clarity. For the R parameter, the DWB2E(g_0) results do not dip as low as the DWB2E(g_{1s}) results at 70° , but the two calculations are qualitatively similar.

We have also looked at the effects of each individual second-order exchange term to determine their relative importance. This comparison revealed that all three terms are comparably important so none of them could be neglected. The first two exchange terms [terms 6 and 7 of Eq. (6)] produce very similar results such that if approximations were necessary, it would not be unreasonable to equate these two terms. This is not particularly surprising in light of the fact that these two terms represent similar physical processes.

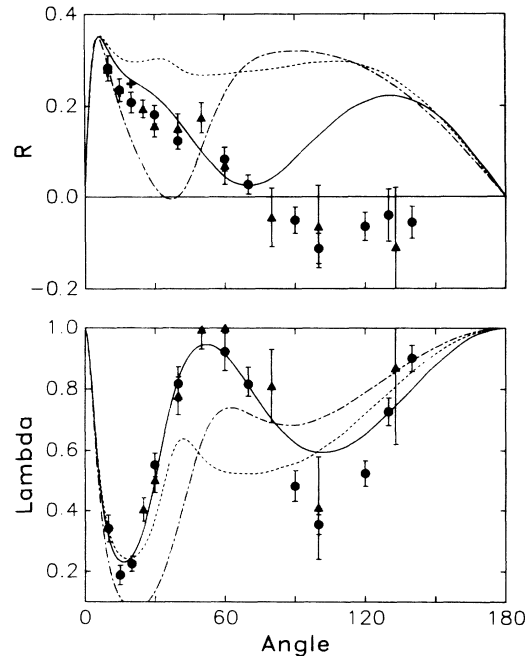


FIG. 2. Angular correlation parameters for 54.4-eV electron-impact excitation of the $2p$ state of hydrogen. The experimental data are from (●) Williams (Ref. 10); (▲) Weigold, Frost, and Nygaard (Ref. 11); and (+) Slevin *et al.* (Ref. 12). The theoretical curves are (dash-dotted line) DWB1; (dotted line) DWB2D(g_0); and (solid line) DWB2E(g_{1s}).

It is to be noted that the differential cross section and λ parameter depend only on the magnitude of the complex T matrix while the R parameter depends on both the magnitude and the phase of the complex amplitude. These results, therefore, indicate that when exchange is included to second order, the resulting T matrices are in good agreement with experiment for the magnitude of the amplitude at all angles and that the theoretical results are in good agreement with the phase of the amplitude for angles less than 60° . Assuming the experiments are correct, the theoretical phases for angles greater than 60° are evidentially incorrect. On this point, it is intriguing and somewhat puzzling that nearly all theoretical calculations predict positive values for the R parameter at large scattering angles while the experimental values are negative. It is also to be noted that Slevin *et al.*¹³ measured the R parameter at 35 eV and they obtained positive values for the R parameter at large scattering angles which are similar to our DWB2E(g_{1s}) results.

The fact that the second-order terms are very important naturally makes one wonder if third- and higher-order terms are also important. This is, of course, an issue of central importance to the utility of perturbation series. For the case of direct scattering, we can get a very good idea of the importance of higher-order terms for elastic scattering by comparing the present results with the optical-model close-coupling calculation of Bray, Madison, and McCarthy.¹⁴ In that calculation, the second-order optical potential was evaluated in the same manner as we have evaluated the second-order amplitude here. Since the Bray, Madison, and McCarthy¹⁴ calculation is a close-coupling calculation, it contains contributions from all orders of perturbation theory. Further, if a perturbation expansion were made of those close-coupling results, the first two terms would be identical to the present calculation. Consequently, the difference between the two calculations represents the effects of a subset of third- and higher-order terms. Comparing the two calculations revealed that the average difference between differential cross sections was 7% at 100 eV and 15% at 54.5 eV. Assuming the close-coupling calculation contains the most important parts of the higher-order terms, these results indicate that the second-order direct scattering term is converged to within (10–15)% for elastic scattering in this energy range. Unfortunately, we cannot make a similar comparison which includes second-order exchange. We would note, however, that the second-order exchange term is of comparable size to the second-order direct term and that the good agreement we have obtained with experiment for three different scattering situations would give a positive indication that the higher-order terms are not important.

In summary, this work is the first perturbation-series

calculation to have included second-order exchange exactly. We found that not only was second-order exchange important, it dramatically improved agreement between experiment and theory for parameters which depended only on the magnitude of the T matrix for three different processes—elastic scattering, $2s$ excitation, and $2p$ excitation. Perhaps the most important consequence of this work lies in the implications for perturbation series. The previous exact second-order results without exchange did not agree with experiment and it was assumed that the problem must originate from third- and higher-order terms. Consequently, it was assumed that it would not be possible to use perturbation series to obtain accurate results because of the extreme difficulty associated with calculating the higher-order terms. These results provide new life for perturbation series since they clearly demonstrate both that second-order calculations are practical and feasible and that accurate results can be obtained from such calculations for the intermediate energy range. A preliminary report of this work was recently presented.¹⁵

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