Full Second-Order Distorted-Wave Calculation without Approximations for Atomic Excitation by Electron Impact

D. H. Madison
Physics Department, Drake University, Des Moines, Iowa 50311
(Received 9 April 1984)

A new technique has been developed for evaluating second-order distorted-wave amplitudes for atomic excitation without making any approximations. By this technique, second-order amplitudes with arbitrary distorted waves and arbitrary Green's functions in the interaction can be evaluated with comparable difficulty. The utility of the method is demonstrated through a practical calculation of the second-order distorted-wave approximation for electron excitation of the $2p$ state of hydrogen.

PACS numbers: 34.10.+x, 34.80.Dp

The technological advances which have occurred over the last several years have created demands for increasingly accurate theoretical cross sections in many areas of physics. Often, results produced by standard first-order perturbation theory are not sufficiently accurate. For such cases, a calculation good to second order in perturbation theory would be highly desirable. While numerous theoretical works have dealt with second-order amplitudes, various simplifying approximations are normally made to make the calculation tractable. For example, in the field of atomic excitation by electron impact, to our knowledge there has been no attempt to evaluate a second-order distorted-wave amplitude exactly without making simplifying approximations. The only previous exact second-order calculation has been the second-order plane-wave Born calculation of Ermolaev and Walters[1] for electron excitation of the $2s$ state of hydrogen.

It would be highly desirable to be able to perform second-order distorted-wave calculations without making approximations since: (1) Approximations always raise questions concerning the validity of the results. (2) Exact results can be used to study and evaluate the various approximations which have been used for the calculation of second-order amplitudes. (3) Through comparison with experimental data, the exact results can be used to determine the importance of the physical effects contributing to the first- and second-order amplitudes and to determine whether there are additional physical effects which are important for a particular scattering situation.

We report here a technique for evaluating arbitrary second-order distorted-wave amplitudes without making any approximations. This technique is outlined in the first part of the paper. In the second part of the paper, the utility of this technique is demonstrated through an application to the problem of electron excitation of the $2p$ state of hydrogen. This problem represents a particularly good test case for the method since there have been many theoretical studies of this problem, and presently agreement between theory and experiment is not particularly good, especially for the alignment parameters. A systematic development and more detailed comparison with experiment and other theoretical calculations will be presented elsewhere.

The second-order distorted-wave amplitude is given by

$$T^2=\sum_{n\neq i,f} T_n^2, \tag{1}$$

with

$$T_n^2=\langle \chi_f^- | V_{fn} g_n^+ V_{ni} | \chi_i^+ \rangle , \tag{2}$$

where $\chi_{i(f)}$ is an initial- (final-) state distorted wave obtained from the initial- (final-) state spherically averaged atomic potential $U_{i(f)}$. We also have

$$V_{mn}=\langle \psi_m | V | \psi_n \rangle , \tag{3}$$

where ψ_k is an atomic wave function for kth state (either discrete or continuum) with energy ϵ_k, V is the full interaction between the incident projectile and the atom, and g_n^+ is the distorted Green's function operator

$$g_n^+=(K_n^2-h_f-U_i+i\eta)^{-1}. \tag{4}$$

Here $K_n^2=E-\epsilon_n$ is the energy difference between the total energy and the energy of the atom in the nth state (i.e., the energy of the projectile when the atom is in state ψ_n) and h_f is the Hamiltonian for the free projectile. It should be noted that the sum in (1) is an infinite sum over all possible discrete and continuum intermediate states and that the initial and final atomic states are excluded from this sum.

The basic problems associated with the evaluation of the second-order amplitude are the infinite sum and the fact that (2) represents a double integral over a nonlocal operator. These problems are generally avoided through simplifying approximations. The first approximation that is made is to replace

the distorted Green's function with the well-known free-particle Green's function [i.e., U_i in (4) is ignored]. Other typical approximations are these: (1) The infinite sum over intermediate states is made by assigning each state the same average energy and by using closure to perform the sum; (2) the distorted waves are replaced by plane waves; or (3) the nonlocal interaction operator is replaced by a local operator.

In the present work, the double integral and problems associated with the nonlocal operator are avoided by defining

$$|\beta_n^+\rangle \equiv g_n^+ V_{ni}|\chi_i^+\rangle, \tag{5}$$

so that

$$T_n^2 = \langle \chi_f^- | V_{fn}|\beta_n^+\rangle. \tag{6}$$

The wave function β_n^+ must satisfy the differential equation

$$(K_n^2 - h_f - U_i)|\beta_n^+\rangle = V_{ni}|\chi_i\rangle, \tag{7}$$

subject to the boundary conditions imposed by g_n^+.

The evaluation of T_n^2 has now been greatly simplified to the solution of a single inhomogeneous differential equation (7) followed by evaluation of a single integral (6). It should be noted that the integral (6) is of the standard form for first-order amplitudes. In fact, if the inhomogenity in (7) is set equal to 0 and $n=1$, β_n becomes χ_i and (6) becomes the first-order distorted-wave amplitude. Consequently, this technique reduces the evaluation of T_n^2 to the level of difficulty of a first-order amplitude. As a result, the full second-order amplitude T^2 becomes a sum of amplitudes of the first-order type. It should also be noted that the Green's function in the interaction (2) now appears in the differential operator of Eq. (7). Consequently, there is no need to make the free-particle Green's function approximation since (7) must be solved numerically and there is no particular advantage in setting $U_i=0$. The basic idea behind this technique is not new,[2,3] but to our knowledge this is the first time it has been applied to inelastic charged-particle scattering.

We have performed a test calculation to determine the time savings represented by (6). The test was performed for electron-hydrogen excitation and a $3p$ intermediate state. The free-particle Green's function approximation was also made so that (2) could be directly evaluated. For this test case, obtaining the second-order amplitude for the $3p$ intermediate state using (6) resulted in a time savings of over two orders of magnitude.

Exact second-order distorted-wave cross sections for electron excitation of the $2p$ state of hydrogen have been calculated to demonstrate the utility of this method. Figures 1 and 2 show the results for the λ parameter, R parameter, and differential cross section (DCS) for 54.4-eV incident electrons. Each figure has the first-order distorted-wave results, first order plus second order including discrete states only in the sum over intermediate states, and first order plus full second order (includes discrete and continuum intermediate states). First-order exchange has also been included in all these results. For the sum over intermediate states, all discrete and continuum states which made an appreciable contribution were included. For the discrete case, all states with $n \leq 6$ and angular momentum states up to and including f states (sixteen in all) were considered. The f states made such a small contribution that they could have been omitted. For the continuum case, 44 different continuum energies corresponding to both open and closed channels between 0.12 and 185 eV were considered. For each of these energies, several different angular momentum states were included. The maximum angular momentum which had to be included for

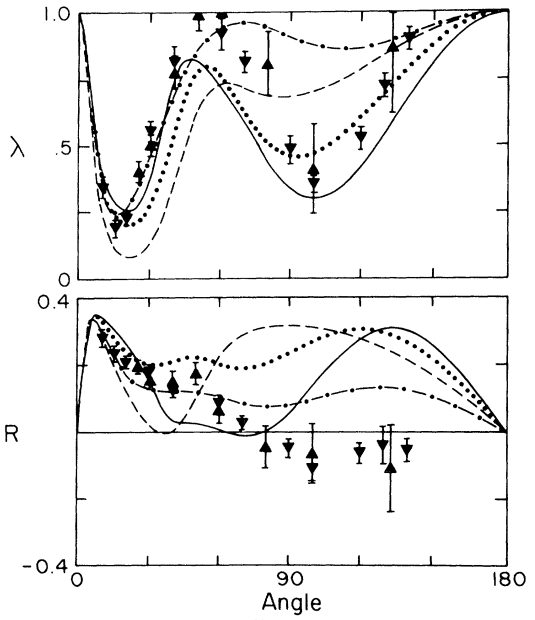

FIG. 1. First- and second-order λ parameters and R parameters for 54.4-eV electron excitation of the $2p$ state of hydrogen. The theoretical calculations are as follows: dashed line, first-order distorted-wave approximation; dotted line, first-order plus discrete part of second-order amplitude; solid line, first-order plus full second-order amplitude; and dash-dotted line, first-order results of Madison *et al.* (Ref. 4). The experimental data are as follows: triangles, Weigold, Frost, and Nygaard (Ref. 5); and inverted triangles, Williams (Ref. 6).

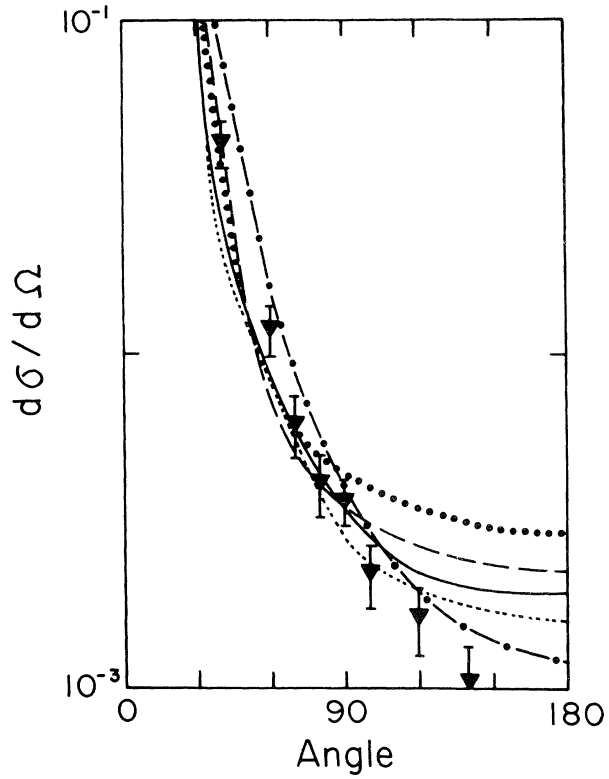

FIG. 2. Same as Fig. 1 except for the differential cross section. The units are a_0^2 and the dashed line represents the closure, second-order distorted-wave results of Kingston and Walters (Ref. 7).

continuum intermediate states ranged between 5 and 8 depending on the energy level. In the end, the contributions from 325 different continuum states were summed and integrated to get the continuum contribution to the second-order amplitude. A partial-wave expansion was made for β_n of (5) and the final-state distorted wave. The number of partial waves required for this expansion depended upon the intermediate state (which determined the long-range behavior) and varied between 12 and 200.

If the first- and second-order distorted-wave results are compared, it is seen that the second-order results are in substantially better agreement with the experimental data than the first-order results. The surprising aspect of the comparison is that the second-order results are still in fairly poor agreement with the data in several instances. If we assume that the experimental data are correct, this relatively poor agreement would indicate that third- and perhaps higher-order effects are fairly important.

It is interesting to compare the second-order results including discrete states only with the full second-order results. It is clear that the continuum part of the spectrum contributes as strongly as the discrete to the final answer. It is also interesting to note that for the λ and R parameters, the discrete contribution moves the results in the direction of the experimental data, while for the large-angle DCS, the discrete contribution moves the results away from the experimental data.

Kingston and Walters[7] have also performed a second-order distorted-wave calculation for this process. The approximations made in the Kingston and Walters work were these: (1) the distorted Green's function was approximated by the free-particle Green's function and (2) the sum over intermediate states was performed by closure. Their results for the DCS are shown in Fig. 2. A detailed comparison of the two second-order calculations shows that the Kingston-Walters approximation gives a DCS that is good to within 10% out to 30° scattering. Beyond 30°, the Kingston-Walters results are too small by generally 13–20% except near 60° where the difference reduces to 5%. At the large angles, the Kingston-Walters closure approximation gives results which are about 15% too small and which fortuitously are in better agreement with the experimental data.

The first-order distorted-wave results of Madison *et al.*[4] are also shown in Figs. 1 and 2. The difference between the present first-order distorted-wave results and those of Madison *et al.* lies in the distorting potential used to calculate the initial- and final-channel distorted waves. The present formalism dictates that the initial-channel distorted wave be obtained from the initial-channel distorting potential U_i, and that the final-channel distorted wave be obtained from U_f. However, it has been known for sometime that if both the initial- and final-channel distorted waves are calculated with use of the final-channel distorting potential U_f, the first-order results are in much better agreement with the experimental data. This procedure, which has become fairly standard, was used in the Madison *et al.*[4] work. To our knowledge, no theoretical justification for this procedure has been given. It is interesting that this first-order calculation is qualitatively in better agreement with the experimental data than the full second-order results.

It is of particular interest to compare the first-order calculation of Madison *et al.*[4] and the full second-order results for the λ parameter in the range of 60–150°, and to note that the full second-order calculation has a rather deep minimum in that region. For the case of excitation of the $2\,^1P$ state of helium, the existing experimental data for the λ

parameter disagree in this angular region. The data of Hollywood, Crowe, and Williams[8] and Slevin *et al.*[9] show a deep minimum similar to the data shown here, while the data of Steph and Golden[10] do not exhibit the deep minimum but rather have the shape of the first-order results of Madison *et al.*[4] The first-order distorted-wave calculation for helium corresponding to the first-order Madison *et al.*[4] results are in good agreement with the Steph and Golden data but not the other two experimental measurements. The present second-order results indicate that a full second-order calculation for helium would exhibit a deep minimum for the λ parameter in this angular range.

In conclusion, the present work demonstrates the feasibility of performing exact second-order calculations with no approximations. For the test case of electron excitation of the $2p$ state of hydrogen, it was found that third- and higher-order effects are important (assuming the experimental data are accurate) and that the closure second-order distorted-wave calculation of Kingston and Walters[7] gives a DCS which is good to within 10% for scattering angles less than 30° and good to within 20% for angles greater than 30°.

The author would like to acknowledge helpful discussions with Y.-K. Kim, J. Macek, and L. Staunton, and computer programming assistance from J. Hughes and D. McGinness. This work was supported by a Northwest Area Foundation grant of the Research Corporation and by the National Science Foundation under Grant No. Phy-8310644.

[1]A. M. Ermolaev and H. R. J. Walters, J. Phys. B **13**, L473 (1980).

[2]A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. London, Ser. A **233**, 70 (1955).

[3]T. N. Chang and R. T. Poe, J. Comput. Phys. **1**, 557 (1973).

[4]D. H. Madison, M. E. Stewart, I. E. McCarthy, and A. Stelbovics, J. Phys. B **16**, 1063 (1983).

[5]E. Weigold, L. Frost, and K. J. Nygaard, Phys. Rev. A **21**, 1950 (1980).

[6]J. F. Williams, J. Phys. B **14**, 1197 (1981).

[7]A. E. Kingston and H. R. J. Walters, J. Phys. B **13**, 4633 (1980).

[8]M. T. Hollywood, A. Crowe, and J. F. Williams, J. Phys. B **12**, 819 (1979).

[9]J. Slevin, H. Q. Porter, M. Eminyan, A. Defrance, and G. Vassilev, J. Phys. B **13**, L23 (1980).

[10]N. C. Steph and D. E. Golden, Phys. Rev. A **21**, 1848 (1980).