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Polarization effect in electron-excitation of hydrogen

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We use the distorted-wave approach in the eikonal approximation to show that polarization effects play a significant role in the direct excitation process of atomic hydrogen by electron impact.

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There is a clear borderline in complexity between close-coupling or R-matrix methods and the T-matrix approach in the theory of atomic collisions. Multichannel methods often provide accurate results but are technically complicated and may be difficult to analyze with respect to physical insight. A low (first) order T-matrix calculation is typically less accurate but technically simpler than the multichannel approach, and may, in a more direct way, reveal the essential reaction mechanisms and identify the most important dynamic elements of the considered process.

The differential cross section and the corresponding angular-correlation parameters for electron excitation of atomic hydrogen at intermediate energies have been considered for a long time to be a cornerstone for the development of atomic collision theory [1]. However, as discussed, for example, by Madison, Bartschart, and Peacher [2] and by Bray and Stelbovics [3], even the most sophisticated theoretical calculations are not in satisfactory agreement with experimental data. The experimental deviation with respect to the calculations of Bray and Stelbovics is particularly puzzling since the latter work is based upon apparently well-converged close-coupling calculations involving an ascending series of up to 80 Laguerre basis states of s, p, d, and f type. The situation is similar when experimental data at intermediate impact energies are compared with theoretical results based upon the distorted-wave approach: There are persistent deviations between theory and experiment, and the inclusion of higher-order effects does not seem to lead to a consistent improvement. As a matter of fact, the elementary first-order distorted-wave approach (DWB1) is not essentially worse in the comparison with experimental data than the most advanced close-coupling method. The DWB1 approximation does, on the other hand, represent a considerable improvement over the plane-wave Born approximation. The inclusion of channel distortion is accordingly important for a proper perturbation treatment. The question is whether the traditional distorted-wave approximation may be significantly improved. Madison, Bartschart, and Peacher [2] noted that the DWB1 approach usually assumes that the distortion potentials are spherically symmetric and proposed that retention of nonspherical distortion potentials might influence the calculations. However, an explicit calculation for the excitation of the $2p$ states of hydrogen appeared to indicate that the effect of nonspherical terms is very small.

In this communication we readdress the problem of nonspherical distortion potentials. First, it is important to recall that the distorted-wave method in its simplest form is determined by the choice of channel potentials. Due to the degeneracy in principal shells, this choice, however, cannot be made in a unique way for the hydrogen atom. There is, accordingly, no unique form of the DWB1 approximation for electron-hydrogen collisions. The form of the DWB1 approximation is not specific until the representation of final states has been chosen. This choice should, preferably, be based upon some sort of physical argument. Considering that the standard correlation parameters refer to atomic states in the angular momentum representation, it is not unnatural to base the DWB1 calculations on distortion potentials pertaining to the spherical representation of final states as done in Ref. [2]. The leading nonspherical term in the distortion potentials is then clearly of quadrupole type. However, Stark states with permanent dipoles are naturally formed when the hydrogen atom is exposed to an electric field or a distant electric charge. The distortion potentials pertaining to such atomic states are of dipole character and thus much stronger than the quadrupole terms pertaining to spherical atomic states. The work reported in Ref. [2] is accordingly inconclusive with respect to the significance of nonspherical terms in the distortion potentials in the T-matrix approach to atomic collisions. As a matter of fact, the present paper will indicate that dipole terms and polarization effects *are* important, in particular with respect to the angular-correlation parameters.

The eikonal DWB1 approximation has been described and used extensively by Joachain and co-workers [4,5]. These authors were concerned with scattering in a lim-

ited forward region, ($\theta \lesssim 25$), and used the so-called "straight-line" approximation. In this approximation the eikonal phase in the initial state as well as in the final state is integrated along a common axis which allows the integral over azimuthal angles in the T matrix to be evaluated analytically. The common eikonal axis is usually taken to be the z axis defined by the momentum, $\mathbf{k_i}$, of the incoming electron. This approximation is obviously without physical meaning for large scattering angles. It would be a much better approximation to integrate the initial phase distortion, U_i, along $\mathbf{k_i}$ and the final phase distortion, U_f, along the momentum of the outgoing electron $\mathbf{k_f}$. However, the numerical evaluation of the corresponding three-dimensional integral for the T matrix is extremely time consuming, and since exchange effects are also expected to become significant at larger scattering angles, we plainly follow Joachain and adopt the straight-line approximation for the calculations reported in the present paper. Our calculations are, accordingly, not expected to be accurate outside a suitable range of forward scattering angles, but this turns out to be sufficient for a qualitative documentation of the importance of the polarization effect. A complete assessment of the effect must await a more extended calculation by one of the established groups in the field. Work in this direction is in progress (Madison and Peacher, private communication). Atomic units are used throughout unless otherwise stated.

The T-matrix element for a direct transition from an initial target state φ_{1s} to a final state, φ_f, with well-defined magnetic quantum number, m_f, is given by the following expression in the eikonal distorted-wave approximation with a common eikonal axis along the initial beam direction [4]:

$$T_f(\theta) = (2\pi)^{-2} \int_0^\infty dbb(-i)^{m_f} J_{|m_f|}(k_f b \sin\theta) \times \int_{-\infty}^{\infty} dz \exp[i(k_i - k_f \cos\theta)z + i\Delta_f(b,z)] A_f(b,z). \quad (1)$$

Here, θ represents the electron scattering angle while the target transition element A_f and the eikonal phase difference Δ are given by the following expressions:

$$A_f(b,z) = \langle \varphi_f(\mathbf{r}') | V(\mathbf{r},\mathbf{r}') | \varphi_i(\mathbf{r}') \rangle \quad (2)$$

and

$$\Delta_f(b,z) = -\frac{1}{k_i} \int_{-\infty}^{z} U_i(b,z')dz' - \frac{1}{k_f} \int_z^\infty U_f(b,z')dz', \quad (3)$$

in terms of the interaction potential

$$V(\mathbf{r},\mathbf{r}') = \frac{1}{|\mathbf{r}-\mathbf{r}'|} - \frac{1}{r}, \quad (4)$$

and the channel distortion potentials ($c = i, f$)

$$U_c(\mathbf{r}) = \int d\mathbf{r}' V(\mathbf{r},\mathbf{r}') |\varphi_c(\mathbf{r}')|^2. \quad (5)$$

Explicit expressions for U_{1s}, U_{2s}, U_{2pm_f}, A_{2s}, and A_{2pm_f} are given in Ref. [4] and shall not be reproduced here.

When the Stark representation is considered the $2s$ and $2p0$ states are mixed in the usual way,

$$\varphi_{2\pm}^{St} = \frac{1}{\sqrt{2}} [\varphi_{2s} \pm \varphi_{2p0}]. \quad (6)$$

The corresponding matrix elements in (1) are then given by

$$A_{2\pm}^{St} = \frac{1}{\sqrt{2}} [A_{2s} \pm A_{2p0}], \quad (7)$$

while the distortion potentials appear in the form

$$U_{2\pm}^{St} = \frac{1}{2} [U_{2s} + U_{2p0}] \pm U_{sp}, \quad (8)$$

where the last term is the dipole contribution alluded to in the introduction,

$$U_{sp}(\mathbf{r}) = \langle \varphi_{2s} | V | \varphi_{2p0} \rangle = 3\frac{z}{r} \left[-\frac{1}{r^2} + e^{-r} \left(\frac{1}{r^2} + \frac{1}{r} + \frac{1}{2} + \frac{r}{6} + \frac{r^2}{24} \right) \right]. \quad (9)$$

In the present work we have evaluated the eikonal distorted-wave amplitudes in (1) for transitions to the $n = 2$ shell in electron-hydrogen collisions at 54.4 eV. Calculations have been performed in the distorted-wave model corresponding to a spherical representation of final states as well as in the distorted-wave model corresponding to a Stark representation of final states. Polarization effects are, accordingly, ignored in the first model but included in the latter. The integrals in (1) must be evaluated numerically. We have tested our program against the results obtained by [4] in the spherical basis, and we have exerted special care to ensure convergence of the integrals at large scattering angles where the phase factors in (1) are rapidly varying.

The differential cross section and the correlation and coherence parameters of relevance in the present connection are expressed in terms of transition amplitudes to the $2p$ manifold of the hydrogen atom. Explicitly, the angular-correlation parameter, λ, and the magnetic-coherence parameters, R and I, are given in the following way in terms of T-matrix elements T_{2pm} for transition to specific sublevels in the spherical basis:

$$\lambda = \frac{|T_{2p0}|^2}{|T_{2p0}|^2 + 2|T_{2p1}|^2}, \quad (10)$$

$$R = \frac{Re[T_{2p0}{}^* T_{2p1}]}{|T_{2p0}|^2 + 2|T_{2p1}|^2}, \quad (11)$$

$$I = \frac{Im[T_{2p0}{}^* T_{2p1}]}{|T_{2p0}|^2 + 2|T_{2p1}|^2}. \quad (12)$$

These expressions may be used directly when the scattering calculations are done in the spherical basis. However, when the Stark basis is used, a coherent superposition is needed to obtain the amplitude for $2p0$ excitation,

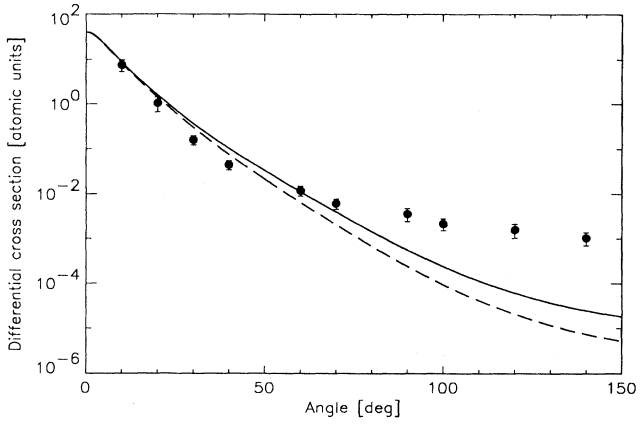

FIG. 1. Differential cross section for $2p$ excitation of hydrogen by electron impact at 54.4 eV. The eikonal distorted-wave theory for direct excitation in the Stark basis of final states is represented by the full-drawn curve. The corresponding theory in the spherical representation of final states is represented by the dashed curve. The experimental data have been adopted from Ref. [6].

$$T_{2p0} = \frac{1}{\sqrt{2}}[T^{St}_{2+} - T^{St}_{2-}]. \tag{13}$$

The calculated differential cross section for direct excitation of the $2p$ level of hydrogen is compared with experimental data in Fig. 1. The comparison is reasonably accurate for scattering angles up to about 70°. This clearly extends beyond the range where the straight-line version of the eikonal approximation can be expected to be accurate. At even larger scattering angles, a distinct divergence between the experimental data and the simple theory sets in. Since it is obviously meaningless to discuss magnitude and phase relations among amplitudes that are known to be absolutely unrealistic, we shall restrict the following discussion to the region of scattering angles below 70°. Notice that the Stark-based differential cross section in Fig. 1 is consistently higher than the cross section obtained when the distorted-wave method is based upon a spherical representation of final states. This difference becomes more pronounced in the correlation and coherence parameters discussed below. The slight departure between the Stark-based cross section and the experimental data is actually due to a deviation in the $|m| = 1$ cross section. This deviation is also apparent in the angular correlation parameter λ shown in Fig. 2. The very pronounced discrepancy between the experimental data and the calculations in the spherical basis actually represents the fact that the theoretical cross section for excitation to the $|m| = 1$ states is overestimated while the $m = 0$ cross section is underestimated. When the polarization effect is included, the $m = 0$ cross section is strongly affected, and the comparison with experiment in Fig. 2 is considerably improved. Note, in particular, that polarization represents a 20% effect in the λ parameter (which, by definition, is restricted to the range between zero and unity). The effect of polarization is similar but somewhat smaller in magnitude when the coherence parameters R and I are considered.

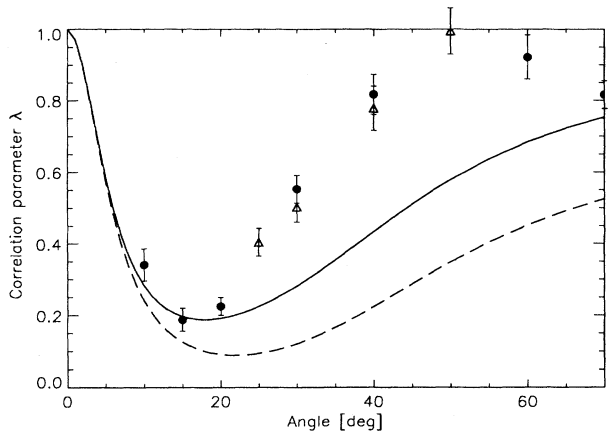

FIG. 2. The angular correlation parameter, λ, for $2p$ excitation of hydrogen by electron impact at 54.4 eV. The notation is similar to Fig. 1: the results in the Stark basis and in the spherical basis of final states are represented by full-drawn and dashed curves, respectively. The experimental data indicated by circles are from Ref. [6] while data from Ref. [7] are marked by triangles.

The available data are shown in Fig. 3, and do not seem to indicate any preference for either of the two types of distorted-wave calculations. The deviation between the two sets of theoretical data is, however, of the same order of magnitude as the deviation between either of the theories and the data. This suffices to provide a qualitative indication of the effect of final state polarization.

Although the present work has been based upon a theoretical approach with a restricted range of applicability, it is implicit to conclude that dipole terms and polarization effects indeed *are* important in the theory of electron impact excitation of atomic hydrogen. This suggests that

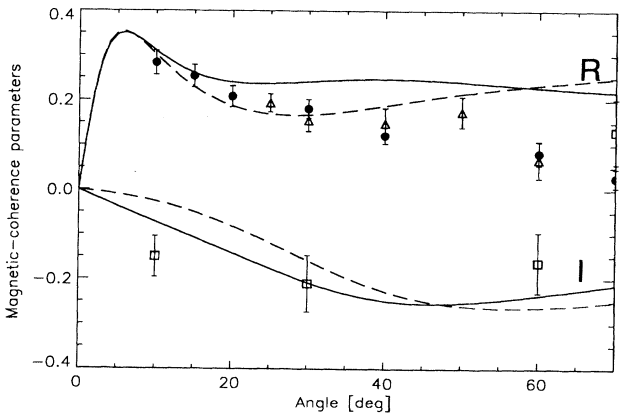

FIG. 3. The magnetic-coherence parameters, R and I, for $2p$ excitation of hydrogen by electron impact at 54.4 eV. The notation is similar to Fig. 1: the results in the Stark basis and in the spherical basis of final states are represented by full-drawn and dashed curves, respectively. The experimental data indicated by circles are from Ref. [6] while data from Ref. [7] are marked by triangles. The data marked by squares are from Ref. [8].

the deviation between experimental data and the "fully converged" close-coupling theory [3] might be due to the neglect of higher angular momentum states, needed to properly model polarization effects in highly excited intermediate states.

It should be noted that the linear Stark effect is peculiar to the hydrogen atom and, accordingly, so is the polarization effect we have been concerned with in this paper. One might therefore consider abandoning inelastic electron scattering from atomic hydrogen as a specially important prototype system if the goal is to test general purpose codes for electron scattering calculations. Note in this connection that Bray [9] recently has demonstrated that large-scale close-coupling calculations for electron-sodium collisions appear to be in excellent agreement with experimental data. The dynamic symmetry property of the hydrogen atom is, on the other hand, so essential that a complete comprehension of its dynamics is a fundamental quest of theory. Further studies of the general dynamics of Coulombic three-body problems should, accordingly, be strongly encouraged. This clearly includes a more quantitative assessment of the effect we have indicated in the present work.

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