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SPIN POLARIZATION IN ELECTRON SCATTERING FROM MOLECULES

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Theoretical results, obtained from the coherent superposition of the waves scattered from the individual atoms, are presented for the spin polarization of 300-eV electrons scattered by C_2H_5I and I_2 molecules, and are found to be in good agreement with experiment.

In a recent Letter, Hilgner and Kessler¹ presented results of the first measurements of the spin polarization of electrons scattered from molecules. They suggested that these polarizations (for electrons of energies of the order of a few hundred electron volts) could be predicted by the coherent superposition of the scattered waves from the individual atoms which make up the molecule. Nonrelativistic calculations have shown that the differential cross sections can be predicted quite accurately using this model, but the calculation of the polarizations requires the scattering amplitudes calculated using the Dirac equation. In this Letter we present the results of two such calculations which show that this model does in fact give results which are in reasonably good agreement with experiment.

The relativistic treatment of the problem follows the same lines as the nonrelativistic approach,² except that the scalar wave functions in the asymptotic forms are replaced by the four-component Dirac wave function

$$\psi_\lambda = a_\lambda e^{ikz} + e^{ikr} u(\theta, \varphi)/r \quad (\lambda = 1, 2, 3, 4). \quad (1)$$

If an average is taken over the possible orientations of the molecule and over the initial spin

polarization of the electron beam, we obtain the expression

$$I(\theta) = \sum_i \sum_j \frac{\sin sr_{ij}}{sr_{ij}} (f_i f_j^* + g_i g_j^*) \quad (2)$$

for the differential cross section, and

$$P_m(\theta) = i \sum_i \sum_j \frac{\sin sr_{ij}}{sr_{ij}} (f_i g_j^* - g_i f_j^*) / I(\theta) \quad (3)$$

for the spin polarization, where f_i and g_i are the relativistic scattering amplitudes for atom i , $s = 2k \sin \frac{1}{2} \theta$, and r_{ij} is the distance between the i th and the j th atoms.

The two cases considered have been scattering from I_2 and C_2H_5I molecules at energies of 300 eV. The atomic scattering amplitudes were calculated using the relativistic Hartree structure and scattering programs developed by Schonfelder.³ In both cases the calculated differential cross sections agreed to within 2% with those measured by Hilgner and Kessler.

The calculated polarizations are shown compared with experiment in Fig. 1. The theoretical polarizations for I_2 [Fig. 1(a)] are the same as those for atomic iodine, and do not depend at all on the interatomic distance. The curve

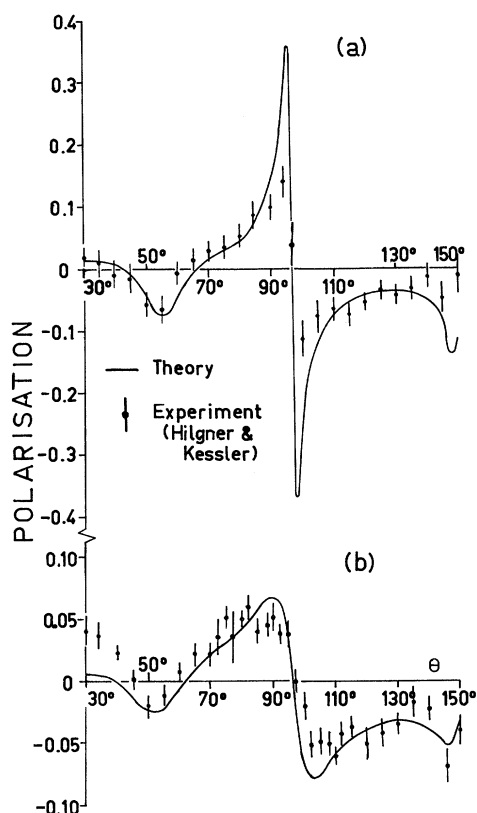


FIG. 1. Spin polarization of 300-eV electrons scattered by (a) I_2 molecules; (b) C_2H_5I molecules, as a function of scattering angle θ .

agrees well with experiment in all except the peak region around 100° , where the observed polarization is less than half that predicted by theory.

For C_2H_5I two models were used, one excluding and one including the hydrogen atoms. The results obtained differed by less than 1%, which is not surprising since the total cross section for atomic hydrogen at this energy is much smaller than those for the other atoms, being 6×10^3 natural units as compared with 4×10^5 for iodine and 9×10^4 for carbon. The results for the simplified model are shown in Fig. 1(b). The theoretical curve again shows a slightly higher polarization than the experimental. Comparison of this with the curve for I_2 demonstrates

very clearly the idea of "dilution" of polarization discussed by Hilgner and Kessler, in which the very small polarization from the carbon atom (the maximum is 0.16%) reduces the resulting polarization, from the molecule as a whole, from the 35% of the iodine atom alone to only 8%. It must be stressed, however, that this effect is due to the carbon atoms only, not to both the carbon and hydrogen atoms as Kessler and Hilgner suggested; since although the electrons scattered from the hydrogen atoms are virtually unpolarized, their contribution to the scattering is negligible.

The differences between theory and experiment could be due to any of the following three causes: (i) errors in the atomic scattering amplitudes; (ii) errors in the interatomic distances used in the calculations; or (iii) modifications in the atomic potentials due to the proximity of the other atoms in the molecule.

The first of these could arise because of exchange effects, the distortion of the atom by the incoming electron, or correlations between the motions of the atomic electrons; but this is unlikely since at this energy these effects are known to be small. The second source of error is irrelevant for I_2 , and in general should be smaller for the polarizations, which depend approximately on the ratios of the interatomic distances, than for the cross sections, which contain them directly and which are in good agreement with experiment. This leaves the final possibility, the modification of the potential due to the presence of the other atoms, as the most probable cause of significant discrepancies. If this is the case, then the polarizations can be used to obtain more information about the precise form of the molecular potential than is possible with the cross sections, which appear to be relatively insensitive to these changes.

¹W. Hilgner and J. Kessler, *Phys. Rev. Letters* **18**, 983 (1967).

²H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Clarendon Press, Oxford, England, 1952), pp. 189-191.

³J. L. Schonfelder, *Proc. Phys. Soc. (London)* **87**, 163 (1966).