Spin asymmetry in electron-impact ionization of hydrogen atoms close to threshold

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I report the results of a calculation of the spin asymmetry in the electron-impact ionization of hydrogen atoms for incident energies between 14 and 20 eV. The work involves a variational close-coupling calculation with a pseudostate basis, supplemented by an optical potential procedure for higher partial waves.

INTRODUCTION

The accurate calculation of the cross section for ionization of atoms by electrons of intermediate energy remains a formidable problem for theoretical physics even in the simplest case in which the atom is hydrogen. Recent measurements of the spin asymmetry in ionization [1,2] focus attention on this aspect of the problem. The cross section for ionization depends strongly on the spin state of the pair of incident and bound electrons. This dependence is described by the ionization asymmetry A,

$$A=\frac{\sigma_I(\uparrow\downarrow)-\sigma_I(\uparrow\uparrow)}{\sigma_I(\uparrow\downarrow)+\sigma_I(\uparrow\uparrow)}=\frac{1-r}{1+3r}\ . \tag{1}$$

Here $\sigma(\uparrow\downarrow)$ and $\sigma(\downarrow\uparrow)$ are, respectively the cross sections referring to antiparallel and parallel orientations of the incident and target electrons, and

$$r=\sigma_T/\sigma_S \tag{2}$$

is the ratio of the cross section in the triplet state to that in the singlet state.

Electron-impact ionization has been studied theoretically by a variety of methods. Reference [2] contains results for A obtained from several calculations by different procedures (However, values for A are not given in some of the references quoted as sources in Ref. [2].) The purpose of the present paper is to report results of a computation of this quantity on the basis of a close-coupling calculation using a basis containing both exact atomic states and pseudostates. I consider electron-impact energies from near threshold to 20 eV, and are able to account reasonably well for the asymmetry.

METHOD

The present calculation follows the procedure described in a previous study of elastic scattering and $n=2$ excitation [3]. The calculation is of the close-coupling type in which the two-body wave function is expanded in a set of states which include both exact atomic states and pseudostates. The set in this calculation contains 11 states (5s-like, 4p-like, and 2d-like functions) of which four are exact (1s, 2s, 2p, and 3d) and the remainder are pseudostates. The parameters of the basis set ("standard 5-4-2") are given in Ref. [3]. The coupled integro-differential equations are solved by a variational method which has been described in detail elsewhere [4], with some modifications mentioned in Ref. [3].

It is essential in the study of ionization by these methods that the channels associated with the pseudostates are allowed to be open. Although the individual pseudostates by themselves have no direct physical significance, each pseudostate is a combination of exact atomic states, including continuum states, and cross sections for the excitation of physical states may be recovered by projection. A calculation of this type was first performed by Gallaher [5]. The procedure I use [6] evaluates the overlap of the pseudostates $|p\rangle$ on the exact bound states $|b\rangle$. The contribution from the bound states implicitly included in the excitation of pseudostates can then be subtracted from the total. The total cross section is obtained from the optical theorem, using the imaginary part of the elastic scattering amplitude. The formula I use is

$$\sigma_I(E)=\sigma_T(E)-\sum_x\sigma_x(E)-\sum_b\left|\sum_p\langle i|t|p\rangle\langle p|b\rangle\right|^2 ,$$

in which σ_T is the total cross section and σ_x is the cross section for elastic scattering or for the excitation of one of the exact bound states incorporated with the pseudostates in the target state basis. In the last term, $\langle i|t|p\rangle$ is the complex amplitude for the excitation of the pseudostate $|p\rangle$ from the initial state $|i\rangle$(1s), and $|b\rangle$ is an arbitrary bound state. Bound states up to $n=100$ are included. Note that if $|b\rangle=|x\rangle$ where $|x\rangle$ is an exact target excited state included in the basis, $\langle p|b\rangle=0$. The quantities $\langle p|b\rangle$ can be computed exactly, using the general expression for a bound state, in terms of hypergeometric functions.

The variational calculations were carried out for $0\le L\le 3$. However, for $L\ge 4$, I used results from another method in which an optical potential derived from a pseudostate basis is added to a six-state close-coupling computation [7]. The optical potential method makes it possible to deduce the total cross section for excitation out of the 1s state. I then make a crude approximation that the ionization cross section is given by this with the excitation cross sections for $n=2$ and 3 states subtracted. At the energies close to threshold we consider, the contribution from these higher partial waves is not large (11%

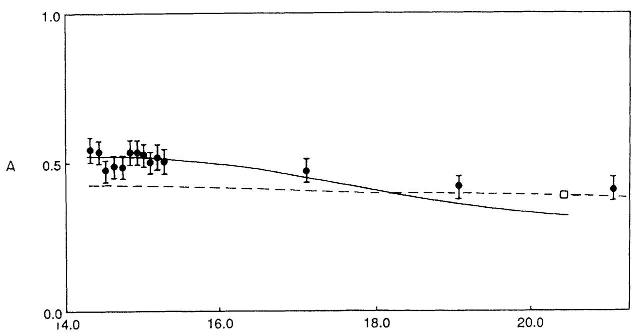

FIG. 1. The spin asymmetry A (dimensionless) is shown as a function of energy. The points with error bars are taken from Ref. [11]. The dashed line shows the results of Ref. [10]. The open square is from the calculation of Ref. [5].

TABLE I. The integrated ionization cross section σ_1 (units πa_0^2) and spin asymmetry A are given for five incident energies.

E (Ry)	$\sigma_I(\pi a_0^2)$	A
1.05	0.045	0.522
1.10	0.066	0.514
1.21	0.112	0.477
1.30	0.157	0.416
1.44	0.244	0.338

at 15-eV incident energies) so the results are not strongly influenced by the rough estimation of the $L \leq 4$ contribution. However, the importance of these partial waves increases with energy. This consideration is one reason why the present work has been limited to impact energies of 20 eV or less (at 20 eV, the contribution from $L \geq 4$ is about $\frac{1}{3}$ of the total).

There is another reason why the calculations are limited to low impact energies. The variational calculation has a broad pseudoresonance in the neighborhood of 30 eV. Above 20 eV, the influence of this pseudoresonance begins to be felt, and the techniques used in Ref. [3] to average over this do not seem to apply readily to the present case, where I am specifically interested in open pseudostates. The lower limit of the energies considered here, $k^2 = 1.05$ (14.28 eV), is just above the thresholds for the $4\bar{s}$, $4\bar{p}$, and $4\bar{d}$ pseudostates that describe the ionization in this energy range.

RESULTS AND DISCUSSION

Our results for the spin asymmetry from 14- to 20-eV impact energies are shown in Fig. 1. Calculations were made at 20 different energies in this range. Representative numerical values are given in Table I.

At the bottom of our range, the total ionization cross section is in fairly good agreement with the measurements of Shah, Elliott, and Gilbody [8], but as the energy increases, the present calculation increasingly underestimates the total. The contributions from the individual partial waves are generally in agreement with the arguments of Greene and Rau [9]. For example, the partial cross section in the ^3S state is much smaller than the others.

The spin asymmetry is seen to be in reasonable accord with the experimental data, particularly in the lower part of the range. The value of the asymmetry extrapolated to threshold is close to $\frac{1}{2}$—that the experimental values are about $\frac{1}{2}$ (instead of 1 which would be the value if only ^1S contributed) was at one time regarded as a great puzzle. The explanation, given by Greene and Rau [9], and supported by these numerical calculations, is that some triplet partial waves for $L > 0$ (particularly ^3P but also ^3F) make a significant contribution at threshold, as also do the ^1P and ^1D waves.

The asymmetry from the present calculations is essentially flat near threshold. I do not find the weak oscillatory structure reported in Ref. [1] in the range between 14- and 15-eV incident energy. There is a clear tendency of the results to fall below experiment near 20 eV.

The underestimation of the total ionization cross section would not imply an incorrect asymmetry if the ratios of singlet and triplet contributions remained correct. However, this does not seem to be the case, and it appears that the ionization in the singlet states is underestimated with respect to that in the triplet state. Analysis of the contributions from the individual partial waves indicates that it is the partial waves of $L \geq 4$, which are not adequately treated in this calculation, that are apparently responsible for the error.

In regard to comparison with other theoretical studies, I consider here only calculations which report directly computed values for A. The energy range I consider here is a difficult one for theory, and has not been extensively studied. A recent calculation of Bray, Madison, and McCarthy [10] derives values of the asymmetry from a one-channel calculation in a weak-coupling approximation (their words: "the DWBA (distorted-wave Born approximation) with the entrance channel calculated in a spin-dependent, complex, nonlocal optical potential"). The asymmetries they report are shown in Fig. 1, and are lower than mine by about 20% close to threshold, but are also somewhat flatter than mine as a function of energy, and are closer than ours to the experimental results from 19 eV on. The only other published theoretical result in this range, due to Gallaher [5], is a value at a single energy (20.4 eV), shown as an open square in Fig. 1.

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