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Electron-impact-ionization cross section for the hydrogen atom

W. Hu, D. Fang, Y. Wang, and F. Yang
T. D. Lee Physics Laboratory, Department of Physics II, Fudan University, Shanghai 200433, People's Republic of China
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A distorted-wave Born exchange approximation was used to calculate the cross section for electron-impact ionization of the hydrogen atoms. Both the integral and energy-differential cross section were calculated. The results were compared with the latest experimental data and other theoretical calculations. Comparison shows that the calculations agree with differential cross-section measurements in general. For integral cross sections the calculation shows a better agreement with an earlier measurement [M.B. Shah, D. S. Elliott, and H. B. Gilbody, J. Phys. B **20**, 3501 (1987)] in which the cross sections are normalized to the first Born approximation.

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I. INTRODUCTION

An electron-atom collision is one of the basic processes in atomic physics. The study of the inelastic electron-atom scattering process is of fundamental importance for the understanding of the physical structure of atoms and molecules and the effects contributing to the collision process. Electron-impact-ionization cross sections are important data in modeling the structure and dynamics of high-temperature plasmas occurring both naturally in stars and artificially in fusion plasma devices. Many efforts have been made both theoretically and experimentally concerning excitation and ionization for ions or atoms [1]. Of all ions and atoms, atomic hydrogen is the simplest example for study. Both experiment and theory can give quite reliable results about the ionization or excitation of hydrogen atoms. For this reason atomic hydrogen attracts the interest of many researchers.

Recently, a new measurement was made of the doubly differential cross section for electron-impact ionization of atomic hydrogen [2]. Discrepancies were found between this and previous measurements and theoretical calculations. Konovalov and McCarthy [3] recently performed a distorted-wave Born approximation (DWBA) calculation for the new measurement. They used two different DWBA methods and found that a calculation including post-collision interaction agrees better in general with the shape of the experimentally measured results. However, the agreement of the calculation with the total cross section is not quite satisfactory.

We have calculated the energy-differential cross sections for some heliumlike ions and the helium atom [4]. In order to test the theoretical method that we used in a previous work, we present in this paper a distorted-wave Born exchange (DWBE) calculation for the case of the hydrogen atom. Both integral and energy-differential cross sections are calculated. The calculation is compared with the new measurement and some earlier experimental data.

II. THEORETICAL APPROACHES

The framework of our DWBE approximation was described in the previous work [4]; the approximation for electron-impact ionization of the hydrogen atom is essentially the same as for electron-impact ionization of positive ions. The total cross section can be written as

$$Q(E_i)=\int_0^{E/2}\sigma(E_e,E_i)dE_e \ , \tag{1}$$

where E_i and E_e are the incident and ejected electron energies, respectively, E is the sum of the ejected and scattered electron energies, and $\sigma(E_e,E_i)$ is the energy-differential cross section.

By using the partial-wave expansion, the calculation of the scattering amplitude can be divided into the calculation of an angular factor and a Slater-type integral. The radial orbitals in the Slater-type integral are solutions of the radial Schrödinger equation (in atomic units),

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}-2V(r)\right]P_l(r)=\varepsilon P_l(r) \ , \tag{2}$$

where l is the angular momentum, ε is the energy of the electron, and $P_l(r)$ is the radial orbital.

Since the object of calculation in this paper is a neutral atom, the Coulomb potential caused by the net charge excess of the ion is not the overwhelming part of the potential. For the incident or scattered electron, the influence of exchange between the free electron and bound electron becomes more important than in the case of ions. In the case of electron scattering from a hydrogen atom, the exchange effects can be treated exactly. In the present work, we used a semiclassical exchange potential [5] to describe the exchange effects. This approximation has been shown to be accurate for low-energy electron scattering from hydrogen atoms. Under such an approximation, the incident or scattered electron experiences a potential

$$V(r)=V_E(r)+V_{\rm SCE}(r) \ , \tag{3}$$

where $V_E(r)$ is the electrostatic potential induced by the charge of the target nucleus and the bound electron and $V_{\rm SCE}$ is the semiclassical exchange potential

$$V_{\rm SCE}(r)=\tfrac{1}{2}(\varepsilon-V_E)-\tfrac{1}{2}[(\varepsilon-V_E)^2+\alpha^2]^{1/2} \ , \tag{4}$$

$$\alpha^2=\frac{2}{r^2}|P(r)|^2\ , \tag{5}$$

where $P(r)$ is the radial orbital of the bound electron.

In this paper, we did not include the post-collision interaction. However, exchange of the two free electrons in the final state was considered, and the maximum interference approximation (MIA) [6] was applied as in Ref. [4].

III. RESULTS

Table I lists the results of the calculation. The calculated energy-differential cross sections are presented as a function of a scaled ejected electron energy x,

$$x=\frac{E_e}{(E_i-I)}\ , \tag{6}$$

where I is the ionization potential. In fact, x is a ratio of the ejected electron energy to the total assignable energy of the two continuum electrons in the final state. It is in the range between 0 and 1. For a given incident energy, the sum of the ejected and scattered electron energies is constant. Since the two electrons in the final state are indistinguishable, the differential cross section $\sigma(x,E_i)$ in Eq. (1) has the following symmetry:

$$\sigma(x,E_i)=\sigma(1-x,E_i)\ . \tag{7}$$

Therefore, we only need to calculate the differential cross sections in the range of $0<x<0.5$.

Figure 1 is the comparison of the experimental [2] and theoretical energy-differential cross sections for different incident energies. For incident energies higher than 60 eV, the calculations agree with the experiment fairly well except at low ejected energies. For $E_i=25$ and 40 eV, the calculated results are slightly higher and flatter than the measurement. The integral (total) cross section is given in Fig. 2, in which the present results are compared with both measurements [7–9] and the calculation of Callaway and Oza [10]. The solid (dashed) curve is the result of calculation with (without) the semiclassical exchange potential V_{SCE}.

Figure 2 also shows that the two curves coincide at high incident energies, which means that the exchange effect between the free electron and bound electron can be neglected at high energies. In fact, this conclusion can also be drawn from the expression of V_{SCE} [Eq. (4)]. The difference between the two curves is substantial at lower energies. At the energies E_i below 50 eV, the dashed curve is much higher than the solid curve at low energies. The solid curve shows a better agreement with experimental data. One can see that inclusion of the semiclassical exchange potential is necessary to improve the calculation, especially at low energies.

In Fig. 2, we can see that the new experimental data are above all the theoretical calculations and the previous measurements at intermediate and high energies. The measurement of Shyn [2] is absolute with an overall uncertainty of about 20% (shown as the typical error bar). The result of Shan, Elliott, and Gilbody [9] is a relative measurement and is normalized to a theoretical calculation of the Born approximation at high energy. Some other even earlier measurements are also plotted in Fig. 2. The discrepancy between these measurements is large. The present results of the total cross sections are between these experiment data, and agree in general with the shape of the new measurement. At higher energies, however, the calculation has a better agreement with the Shah measurement.

Callaway and Oza used a combination calculation of the variational pseudostate (total angular momentum $L\le 3$) and close coupling ($L>3$) methods. Their results show good agreement with Shah's measurement at low energies. The recent theoretical calculation of Konovalov and McCarthy [3] gives a result for the total cross section similar to the present work, but their result is closer to our calculation without the exchange potential. The authors of Ref. [3] suggest that the post-collision interaction is important in DWBE calculations. From Fig. 1 of Ref. [3], one can see that inclusion of post-collision effects did improve the calculation at low incident energy ($E_i=25$ eV). The present calculation shows a reasonably good agreement with the measurement. From Fig. 1 of

TABLE I. Energy-differential cross sections (cm^2/eV) and integrated cross sections (cm^2). The numbers in brackets denote multiplicative powers of ten.

x \ E_i (eV)	25	40	60	100	150	250
0.01	1.67[−17]	1.43[−17]	1.15[−17]	7.66[−18]	5.20[−18]	3.00[−18]
0.05	1.42[−17]	1.10[−17]	7.68[−18]	4.14[−18]	2.17[−18]	8.03[−19]
0.10	1.19[−17]	8.43[−18]	5.07[−18]	2.19[−18]	9.57[−19]	2.82[−19]
0.15	1.03[−17]	6.62[−18]	3.60[−18]	1.33[−18]	5.19[−19]	1.36[−19]
0.20	9.11[−18]	5.29[−18]	2.64[−18]	8.76[−19]	3.16[−19]	7.81[−20]
0.25	8.21[−18]	4.36[−18]	2.01[−18]	6.14[−19]	2.11[−19]	5.00[−20]
0.30	7.50[−18]	3.72[−18]	1.60[−18]	4.56[−19]	1.51[−19]	3.49[−20]
0.35	6.97[−18]	3.26[−18]	1.33[−18]	3.59[−19]	1.15[−19]	3.61[−20]
0.40	6.59[−18]	2.95[−18]	1.16[−18]	3.01[−19]	9.49[−20]	2.11[−20]
0.45	6.37[−18]	2.77[−18]	1.06[−18]	2.69[−19]	8.39[−20]	1.85[−20]
0.50	6.30[−18]	2.72[−18]	1.03[−18]	2.59[−19]	8.03[−20]	1.76[−20]
Int.	5.27[−17]	7.50[−17]	7.52[−17]	6.30[−17]	4.96[−17]	3.35[−17]

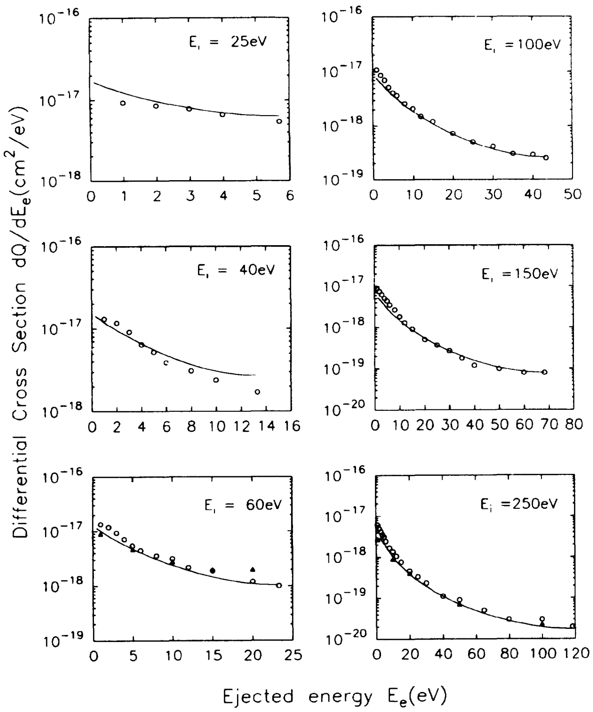

FIG. 1. Energy-differential cross sections for electron-impact ionization of atomic hydrogen at different incident energies. Solid curve is present calculation, open circles are experimental measurements of Shyn [2]. The filled triangles in the bottom two figures are theoretical results from Konovalov and McCarthy [3].

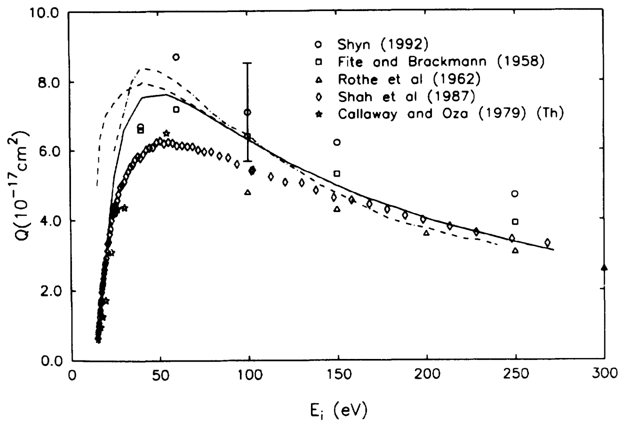

FIG. 2. Total cross section for electron-impact ionization of atomic hydrogen. Solid and dashed curves are the present calculations. The solid (dashed) line is the calculation with (without) exchange potential, the dot-dash curve is the theoretical result of Konovalov and McCarthy [3]. All points except ☆'s are experimental data [2,7–9]. ☆'s are theoretical calculation of Callaway and Oza [10].

this paper, one can see that the discrepancy of theoretical and experimental results is mainly at low ejected electron energies. In other words, the disagreement occurs when the energies (velocities) of the two final free electrons are different. Under such circumstances, the interaction of two electrons should be weaker than the case when the two electrons have about the same energy (velocity). If this is correct, the discrepancy may not be primarily caused by post-interaction effects. We noticed that Ref. [3] did not consider exchange effects on the two final electrons. We performed a separate calculation without exchange of the final electrons. The result is much higher than that including the exchange effects, though the shape of the differential cross sections is about the same. This indicates that exchange between the two continua in the final state is crucial in the calculation. We must emphasize that we used MIA to treat the exchange effects. There is no reason to choose such an approximation other than that it gives better agreement with the experimental results. However, this is not always the case. We previously found that the natural phase approximation is better for boronlike ions [11].

IV. CONCLUSION

In this paper, electron-impact-ionization cross sections for atomic hydrogen are calculated using the DWBE approximation. Both the energy-differential cross section and total cross section of the present calculation are compared with recent experimental data. Comparison was also made with some previous measurements and other calculations. The calculated differential cross sections agree in shape with the measurement. The integral cross section is between the new measurement and older experimental results. In the calculation, we also found that inclusion of a semiclassical exchange potential is necessary to improve the calculation at low incident energies.

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