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Positron impact ionization of atomic hydrogen

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In recent experimental work, the integrated ionization cross section for positron impact on atomic hydrogen has been obtained in the energy range from threshold to several hundred electron volts. All previous theoretical calculations for this process are found to lie well below the measured values. Within the framework of the distorted-wave approximation, we consider improvements to the description of the interaction between the two outgoing particles. This interaction is described in terms of effective charges while distortion in the incident channel is also included. Good agreement is obtained with experiment.

1. Introduction

In a recent experiment, Spicher et al. [1] determined absolute values of the integrated ionization cross section for positron collisions with hydrogen atoms. These measurements represent the cross section for true ionization, that is, positronium formation is not included. The e^+–H system is of particular interest, as compared to the e^-–H system, since it contains three distinct particles and hence exchange of identical particles is not possible. Because of the simplicity of the system, it represents an ideal test for theoretical models of the ionization process.

Earlier measurements on positron ionization of *helium* atoms were carried out by Fromme et al. [2]. Campeanu et al. [3] studied this process theoretically using a number of distorted-wave models which included the effects of distortion and screening in the final channel. Two of these models produced satisfactory agreement between the experimental data and the calculated values. However, when these models were applied to the positron–hydrogen system by Mukherjee et al. [4,5] they yielded values for the integrated ionization cross section which were substantially below the experimental results. Similar work by Ghosh et al. [6] and Hsu et al. [7] also produced theoretical results well below experiment, as did the classical trajectory calculations of Ohsaki et al. [8] and Wetmore and Olson [9]. Thus, the important question arises as to whether there is a fundamental discrepancy between theory and experiment for this simple system or whether a more elaborate theoretical investigation will resolve the issue.

2. Theory

Here we address the problem by employing models which involve a more detailed description of the interaction between the two outgoing particles and the residual ion. We thereby provide a more realistic description of the ionization process than was the case in previous work. The free particles in the final channel are described as moving in the field of energy dependent effective charges situated at the nucleus [10,11].

If the interaction potential in the final channel is described by V_β, then the exact scattering amplitude (in atomic units) is given by the integral expression

$$f(\boldsymbol{k}_e, \boldsymbol{k}_f) = -(2\pi)^{-5/2}\langle \Phi_\beta(\boldsymbol{r}_1, \boldsymbol{r}_2) | V_\beta | \Psi_\alpha^+(\boldsymbol{r}_1, \boldsymbol{r}_2)\rangle$$
$$= -(2\pi)^2 T_{fi}\,. \tag{1}$$

The coordinates of the positron are denoted by $\boldsymbol{r}_1$, and those of the atomic electron by $\boldsymbol{r}_2$. The incident projectile has momentum $\boldsymbol{k}_i$, and therefore its kinetic energy is $E_i=\frac{1}{2}k_i^2$, in atomic energy units. The scattered projectile and the ejected atomic electron have momenta $\boldsymbol{k}_f$, $\boldsymbol{k}_e$ and energies E_f, E_e respectively. Ψ_α^+ is the exact wavefunction with an incident plane wave in channel α and outgoing wave boundary conditions. Similarly, Φ_β is the wavefunction in channel β when the interaction potential is set to zero. The form of the potential is discussed in detail below. The integrated cross section formula for positron impact on hydrogen is given in terms of the scattering amplitude by [12]

$$Q(E_i)=\frac{1}{k_i}\int_0^{E_i-\mathrm{IP}} k_f k_e \,\mathrm{d}(\tfrac{1}{2}k_e^2) \times \iint |f(\boldsymbol{k}_e,\boldsymbol{k}_f)|^2 \,\mathrm{d}\hat{\boldsymbol{k}}_e \,\mathrm{d}\hat{\boldsymbol{k}}_f \,, \tag{2}$$

where IP denotes the ionization potential of atomic hydrogen. From energy conservation one obtains the relationship

$$k_i^2=k_f^2+k_e^2+2\,\mathrm{IP}\,. \tag{3}$$

By taking the initial channel as α and the final channel as β, we can decompose the total Hamiltonian H as

$$H=H_\alpha+V_\alpha=H_\beta+V_\beta\,. \tag{4}$$

The initial channel interaction potential between the incident positron and the hydrogen atom is given by

$$V_\alpha=1/r_1-1/r_{12}\,, \tag{5a}$$

so that the non-interaction wavefunction in the initial channel is $\Phi_\alpha=\exp(\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}_1)\psi_b(\boldsymbol{r}_2)$ where ψ_b is the wavefunction for the hydrogen atom in its ground state. In the final channel the interaction involves the free electron and positron in the field of the proton and hence is given by

$$V_\beta=1/r_1-1/r_2-1/r_{12}\,. \tag{5b}$$

We base our distorted-wave treatment of the ionization process on the two-potential form of the T-matrix [13],

$$T_{fi}=\langle\Xi_\beta^-\,|\,V_\alpha-W_\beta\,|\,\Phi_\alpha\rangle+\langle\Xi_\beta^-\,|\,W_\beta\,|\,\Psi_\alpha^+\rangle\,. \tag{6}$$

Here the potential in the final channel is written as $V_\beta=U_\beta+W_\beta$ and the distorted waves Ξ_β^- are the eigenfunctions of $H_\beta+U_\beta$. We remark that eq. (6) is exact for any choice of U_β. We now replace the exact wavefunction Ψ_α^+ by a distorted wave $\Xi_\alpha^+(\boldsymbol{r}_1,\boldsymbol{r}_2)$ which is an eigenfunction of the distorted Hamiltonian $H_\alpha+U_\alpha$ with some appropriate choice of the distortion potential U_α. With this substitution the T-matrix is no longer exact and the accuracy of the approximate T-matrix depends on the particular choices made for U_α and U_β. Campeanu et al. [3] found that the cross section results were not very sensitive to the chosen form of U_α but depended more crucially on U_β. Here we choose U_α to be a potential that depends only on r_1 and is the sum of the static potential of the hydrogen atom plus the Bethe–Reeh dipole polarization potential [14]. Thus Ξ_α^+ is the product of the hydrogen ground state wavefunction times a distorted wave representing the incoming positron which we denote by χ_i. For the final channel we choose U_β to be of the general form

$$U_\beta=\frac{z_f}{r_1}+\frac{z_e}{r_2}\,, \tag{7}$$

where the effective charges z_f and z_e are independent of the coordinates of the particles but are allowed to depend parametrically on the energies of the scattering and ionized particles. Consequently, if $\phi(z,\boldsymbol{r})$ is the regular Coulomb function with charge z, then

$$\Xi_\beta^-(\boldsymbol{r}_1,\boldsymbol{r}_2)=\phi_f(z_f,\boldsymbol{r}_1)\phi_e(z_e,\boldsymbol{r}_2)\,. \tag{8}$$

With theses choices the T-matrix given in eq. (6) becomes, after some simplification,

$$T_{DW}=\langle\Xi_\beta^-\,|\,V_\alpha\,|\,\Xi_\alpha^+\rangle - \langle\phi_e\,|\,\psi_b\rangle\langle\phi_f\,|\,U_\alpha\,|\,\chi_i\rangle\,. \tag{9}$$

The first integral is the form of the T-matrix commonly used in ionization. We note that the second term is zero if ϕ_e is a Coulomb function with charge unity.

Jetzke and Faisal [10] have shown that it is possible to separate the interaction potential of an N-particle system into a sum of Coulomb interactions with energy dependent effective charges in the asymptotic region. They have used this form of the interaction potential to calculate triple differential cross sections for the ionization of hydrogen by electrons and positrons. Whelan et al. [11] have also used these effective charges in their study of electron ionization of hydrogen. We have adopted this choice of effective charges for the present work. Specifically they are given by

$$z_e = -1 - \frac{(\boldsymbol{k}_e - \boldsymbol{k}_f)\cdot\boldsymbol{k}_e}{|\boldsymbol{k}_e - \boldsymbol{k}_f|^3} k_e\,, \tag{10a}$$

$$z_f = 1 - \frac{(\boldsymbol{k}_f - \boldsymbol{k}_e)\cdot\boldsymbol{k}_f}{|\boldsymbol{k}_e - \boldsymbol{k}_f|^3} k_f\,. \tag{10b}$$

We note that these charges satisfy the Peterkop–Rudge–Seaton (PRS) condition

$$\frac{z_e}{k_e} + \frac{z_f}{k_f} = -\frac{Z}{k_e} + \frac{Z}{k_f} - \frac{1}{|\boldsymbol{k}_e - \boldsymbol{k}_f|}\,, \tag{11}$$

which is a rigorous asymptotic condition that applies to the ionization problem [15,16]. We also note that the singularity that occurs when $\boldsymbol{k}_e = \boldsymbol{k}_f$ is a reflection in the energy domain of the singularity in the interaction potential $1/r_{12}$ which occurs when $\boldsymbol{r}_1 = \boldsymbol{r}_2$. This singularity is also implicit in the PRS condition. These singularities produce no numerical difficulties in the calculation of the scattering amplitudes as the Coulomb functions are well behaved as the effective charges go to $\pm\infty$.

In order to make the calculation of the integrated cross sections (2) tractable, we have evaluated the effective charges by assuming that $\boldsymbol{k}_e$ and $\boldsymbol{k}_f$ are parallel which thereby yields

$$z_e = -1 + \frac{k_e^2}{(k_f - k_e)|k_e - k_f|}\,, \tag{12a}$$

$$z_f = 1 - \frac{k_f^2}{(k_f - k_e)|k_e - k_f|}\,. \tag{12b}$$

However, we do not carry this assumption over to the evaluation of the scattering amplitudes and cross sections which have the full angular dependence on the direction of the particles in the final channel.

3. Results and conclusions

In fig. 1 we show our values of $Q(E_i)$ for positron impact ionization of atomic hydrogen as determined by our model which we denote by EDEC. We have used a 20 point Gaussian quadrature in the energy integral. The partial wave amplitudes were calculated for increasing values of the angular momenta

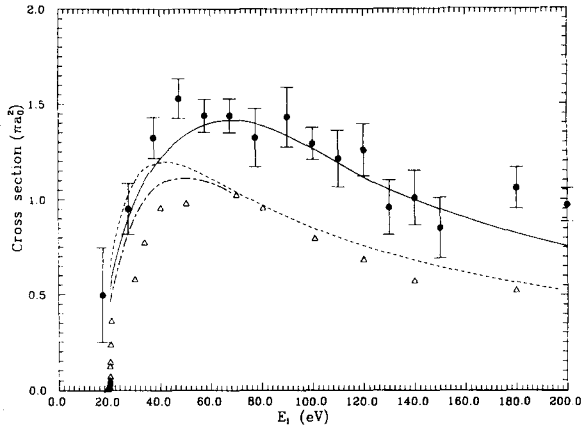

Fig. 1. Integrated ionization cross section for atomic hydrogen by positron impact. (●) Experimental results [1]. Theoretical results: (——) present results, EDEC; (△) ref. [9]; (- - -) ref. [5], DW2; (- - -) first Born approximation.

until they converged to the Born values within a set tolerance. The Born values were then used for the higher partial wave amplitudes via a subtraction technique employing the closed form for the Born amplitudes [16]. Also shown are the experimental measurements of ref. [1], the first Born approximation as calculated from the closed form for the scattering amplitudes and the theoretical calculations of refs. [5,9]. The results of ref. [6] are very close to the Born values, while the distorted-wave calculations of refs. [4,7] lie in the same range as those of ref. [5]. The classical trajectory cross sections of ref. [8] lie slightly below those of ref. [9].

In comparison with the experimental data, our results lie mostly within the error bars in the intermediate energy range. At higher energies we seem to fall below the experimental measurements. However, we expect that the ionization cross section should approach the first Born approximation in the high energy limit. Spicher et al. took measurements up to energies of 600 eV and their values approach the Born results at those higher energies. Thus their points located at approximately 180 eV and 200 eV do not accurately reflect the high energy behaviour of the data.

We note that the agreement between experiment and theory for the integrated ionization cross sections of atomic hydrogen by positron impact has been improved by using the energy dependent charges

[10,11] to describe the interaction of the particles in the final channel. Thus the disagreement between the experimental results and the previous theoretical calculations would seem to reflect the particular choice of model used for these calculations and does not represent a fundamental disagreement between theory and experiment. More elaborate calculations on this system are required to provide a definitive answer to this question.

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