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An investigation of the scaling of plane-wave born cross sections for positron-H_2 considering the positronium-formation channel

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ABSTRACT

Cross sections for positron-H_2 scattering using positronium formation have been studied using the scaled plane-wave Born approximation, originally proposed by Kim [Y. K. Kim, Phys. Rev. A **64**, 032713 (2001)] for electron scattering. The modified scaling for positron scattering is simpler than the scaling for electron scattering. Moreover, the former converts the present first Born approximation into accurate results comparable to the convergent close coupling results. Comparisons to available theoretical and experimental data on positron-H_2 scattering are presented.

1. Introduction

Knowledge of positronium (Ps) formation cross sections and the effect of the Ps-formation channels on other scattering channels have been well studied for atomic targets [1,2]. For molecular targets, although there exist specific measured data for the, for example, Ps-formation cross sections in positron-H_2 scattering [3,4], theoretical calculations for the same are not in a very advance state. The theoretical ground-state Ps formation in the simplest hydrogen molecule was first considered by Sural and Mukherjee [5] using a approximate form of the first Born approximation (FBA), Bussard et al. [6] gave a estimate of the low-energy total Ps-formation cross sections in the positron-H_2 scattering using a indirect method by fitting values to match with Sural and Mukherjee [6], and Biswas and Ghosh using a second Born approximation [7,8]. Multicentredness of the molecular target is the main stumbling block in performing any quantal calculation on it. The inclusion of the Ps formation adds one more centre to the problem. Moreover, due to the multicentredness of the molecule, one is required to perform an averaging over the molecular orientations, i.e. integration over two more dimensions. Obviously, the dimension of the problem suggests that some suitable approximation be made in formulating the theoretical model for the positron-molecule scattering, particularly when the Ps-formation channel is considered. Experimentally, the Ps-formation cross sections in positron-H_2 scattering were measured by Fornari et al. [9], Griffith [10], and Fromme et al. [11]. The scaling method for electron scattering was developed by Kim [12] and use a simple formula to convert FBA excitation cross sections into reliable cross sections comparable to the most accurate theoretical or experimental data available for dipole-allowed transitions. The FBA cross sections can use uncorrelated wave functions, and the scaling requires only the binding energy "B" of the electron being excited, the excitation energy "E_{exc}", and an accurate dipole oscillator strength "f" for the transition (a great success for excitation and ionization cross sections of atoms and molecules was obtained at last years using this method [13–15]).

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Although the model presented by Kim [12] can generate quite accurate integral cross sections which compare well with experimental data the model has some inherent limitations owing to its relatively simple origin. The cross sections using FBA for simple atoms or molecules have been calculated since computers became powerful enough to perform such calculations, but it is now rare to find a paper on Born cross sections for electronic excitations of targets. This therefore represents a possible impediment in the implementation of the "scaling Born approach". Some studies using the scaling Born approach illustrates that the method could never hope to supplant *ab initio* scattering calculations, it simply cannot provide a mechanistic description of the scattering process. Nevertheless where such calculations are impractical or unavailable at this time, the scaling Born procedure for electron scattering does offer a very useful alternative. Cross sections for positron and electron impact are virtually identical at high energies and if the basic dynamical ingredients for this evidence is the FBA, then is possible extend the analysis developed by Kim [12] to more complicated systems as positron-atom or positron-molecule scattering. This is a important consideration and can be significant for studies using positron as incident particle. The goal of the present scaling method is to provide a simple theoretical method to calculate excitation cross sections for positron-molecule scattering using the scaled Born approximation.

In Sec. 2 we identify changes necessary to transform the model proposed by Kim [12] and the present model for positron scattering. In Sec. 3 we discuss the application of the method for e^+-H_2 scattering. Conclusions are presented in Sec. 4.

2. Theory

The FBA is used as the starting point in the present work because (a) the plane wave is the correct wave function at infinity for an positron colliding with a target, and (b) it is the simplest collision theory that uses target wave functions explicitly. Qualitatively the FBA does not account the distortion of plane wave in the vicinity of the target, or the polarization of the target due to the presence of the incident positron. The scaling method proposed by Kim [12] for electron scattering combine these deficiencies into simple functional forms that depend on a few target properties. Here, we will verify that for positron scattering these deficiencies also are combined. In a generic form, FBA cross sections σ_{Born} for inelastic collisions are written as [13].

$$\sigma_{\text{Born}} = [(4\pi aR)/E_o]f_{\text{Born}} \tag{1}$$

where α is the Bohr radius, R is the Rydberg energy, E_o is the incident positron energy, and F_{Born} is the collision strength. The scaling method proposed by Kim [12], referred to as BE scaling, can be written as [12].

$$\sigma_{BE} = [E_o/(E_o + (B + E_{\text{exc}}))]\sigma_{\text{Born}}(E_o) \tag{2}$$

where replaces the E_o that appears in the denominator of Eq. (1) by $E_o + B + E_{\text{exc}}$, and B represent the ionization energy, or the binding energy, of the target electron, and E_{exc} is the excitation energy. The scaling method proposed here for positron scattering is similar to the scaling method of Kim [12] and now replaces the E_o that appears in the denominator of Eq. (1) by $(E_o + E_{\text{Ps}} + E_{\text{exc}})$ where E_{ps} is the positronium energy, and E_{exc} is the excitation energy. The new scaling method by positron scattering is introduced as

$$\sigma_{\text{positron}} = \left[E_o/\left(E_o + \left(E_{\text{ps}} + E_{\text{exc}}\right)\right)\right]\sigma_{\text{Born}}(E_o) \tag{3}$$

with the argument that the effective kinetic energy of the incident positron see by the target is E_o plus the positronium energy (that represent the incident positron attracted by the electron of target), and excitation energy E_{exc}. At present, the Eq. (3) cannot be "derived" from first principle and the combination $E_{\text{ps}} + E_{\text{exc}}$ not be taken literally as a rigid rule, but only as an indicator of the order of magnitude of a constant shift to be added to E_o. Validating a scaling method for Born cross sections (σ_{Born}) of molecules requires two initial ingredients: (i) the Born integral cross sections themselves; (ii) reliable experimental or theoretical optical oscillator strengths. The *f*-scaling proposed by Kim [12] is based on the ratio of an accurate *f* value to a less reliable *f* value produced by the target wave functions actually used to generate $\sigma_{\text{Born}}(E_o)$.

$$\sigma_{[BEf]} = (f_{\text{accur}}/f_{\text{Born}})\sigma_{BE} \tag{4}$$

and our scaling method can be written as

$$\sigma_{f-\text{positron}} = (f_{\text{accur}}/f_{\text{Born}})\sigma_{\text{positron}} \tag{5}$$

We consider here the formation of the Ps atom in its ground state in positron-H_2 scattering. In case of targets with two electrons a Ps atom may be formed with either of the electrons of the target. To calculate the cross section properly, one does require to consider the spin of the system. It has been shown by Mondal et al. [16] that in the case of Ps formation from two-electron system in a singlet spin state, the cross sections may be obtained without explicitly considering the spin and that the probability of ortho-Ps formation is tree times greater than of the para-Ps formation. Without explicitly considering the spin the FBA scattering amplitude for the para-Ps formation in e^+-H_2 scattering was written by Lino [17] where physical cross sections which depend on $f^{\text{FBA}}(k_i,k_f)$ are obtained by taking an average of amplitude over arbitrary molecular orientations (σ_{Born}) [17]. To the best of our knowledge, our cross sections will be the first estimate positron-H_2 scattering (for Ps formation)