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Study of the electron–electron correlation via observing the two-electron cusp

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ABSTRACT

In a recent experiment we found evidence for the existence of the two-electron cusp in atomic collisions, i.e. the enhanced simultaneous emission of two electrons in forward direction with velocities equal to that of the projectile. In the experiment the energies of the two electrons resulting from the mutual target and projectile ionization in 100 keV He^0 + He collisions were measured. The strong correlation observed between the energies of the electrons was explained by an angular correlation of 180° in the projectile-centered reference system. For the interpretation of the experimental results we carried out a Monte Carlo simulation based on the Wannier theory for the two-electron break-up process at threshold. In the article we review the details of the simulation and present two extensions of the model: One takes into account the post-collisional interaction (PCI) between the outgoing electrons and the ionized target atom, while the other contains a correction for a two-center effect.

1. Introduction

The correlation between two low-energy electrons emerging from the near-threshold single ionization of a stationary target atom by electron impact (or double ionization by photon irradiation) has been subject of numerous experimental and theoretical studies in the past decades. It was Wannier [1] who showed for the first time in 1953 that at the threshold the two-electron break-up is a highly correlated process, in which the electrons move symmetrically in opposite directions. Wannier's analysis was based on the general threshold laws derived by Wigner [2] who recognized that the energy dependence of the cross section of a collision process in the neighborhood of a threshold energy is governed only by the type of the interaction (long- or short-range, attractive or repulsive), and it is not influenced by the detailed dynamics of the collision. This universality of the threshold laws explains the large number of investigations carried out for threshold processes (see [3] for a review).

Wannier's prediction of the highly correlated electron emission is strictly valid at the threshold. This means that for an efficient check of the theory one has to measure the angular correlation between the escaping electrons at very small electron energies. As an example, we mention the recent accurate experiment carried out by Williams et al. [4] for electron-impact ionization of hydrogen in which the authors measured the angular and energy correlations of the outgoing electrons down to 0.05 eV.

In the field of energetic ion-atom collisions a unique possibility to observe extremely low-energy (~ meV) electron emission is provided by the so-called cusp phenomenon. The cusp is a peak appearing in the energy spectrum of the electrons emitted from the collision in forward direction. The electrons contributing to the cusp move with velocities approximately equal to that of the bombarding ion (atom), i.e. they fly with very small velocities relative to the projectile. Therefore, an electron spectroscopic experiment performed for the cusp can be regarded as a 'moving laboratory' experiment by which one can obtain information about the properties of the low-energy electron emission in the projectile-centered reference system. The cusp formation is a threshold phenomenon when it is viewed in the projectile frame: Electrons emitted with small positive energies populate low-lying continuum states around the projectile, while those having small negative energies occupy projectile-centered bound states characterized by large principal quantum number (Rydberg states). For single-electron emission the dominant role in the cusp formation is played by the electron–projectile interaction, therefore the process is governed by two-body threshold laws. Among others the threshold character of the cusp explains the continuous interest towards this phenomenon since its discovery [5]. With an appropriate choice of the collision system, by measuring the cusp one can obtain information about the threshold laws for various types of interactions (Coulomb, dipolar, short-range, see, e.g. [6]).

On the basis of the universality of the threshold processes one may assume that the Wannier-type correlated two-electron states can also be formed in ion-atom collisions. A natural candidate for a process leading to such final states is the formation of the two-electron cusp via simultaneous emission of two electrons in

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forward direction with velocities equal to that of the projectile. In the projectile-centered reference frame the electron pairs occupy low-lying two-electron continuum states. Due to the small electron energies, these states are expected to be highly correlated. To observe the two-electron cusp, recently we carried out an experiment [7] in which we measured the energies of the two electrons resulting from the simultaneous target and projectile ionization in 100 keV He^0 + He collisions by detecting triple coincidence between the electrons and the outgoing He^+ ion. The coincidence yield was found to peak at the expected cusp position as a function of the electron energies, giving evidence for the existence of the two-electron cusp. Furthermore, we observed a strong correlation between the electron energies in the vicinity of the cusp which was explained by an angular correlation of 180° in the projectile frame. We performed a Monte Carlo simulation of the process in which the correlated motion of the electrons was taken into account according to the Wannier theory. As a result of the simulation we established that the prediction of the latter theory was consistent with the observed correlation.

In [7] our Monte Carlo simulation was only briefly discussed. In this paper we present the details of the calculation, and compare the results of the simulation with the experimental data more thoroughly. Furthermore, we extend the model by including the post-collision interaction (PCI) between the electrons and the ionized target atom, as well as we develop a simple correction procedure in which the change of the angular correlation between the electrons as a result of a two-center effect is taken into account.

2. Monte Carlo simulation based on the Wannier theory

A disadvantage of a moving laboratory experiment is that it provides indirect information about the electron emission, i.e. the obtained data cannot be compared directly with the predictions of a theory. To make a comparison between theory and experiment, one has to transform the theoretical electron emission cross sections from the projectile frame to the laboratory frame by a velocity (Galilean) transformation and then integrate the resulting cross sections in the velocity space over the detection volume determined by the acceptance angles and energy resolutions of the electron detectors. For a comparison between theory and experiment we chose an alternative way, namely the Monte Carlo simulation of the electron emission. We randomly create individual electron trajectories with the theoretically predicted energy and angular distribution, and track the path of the electrons until they reach the detectors. Using this method, the experimental conditions of the electron detection can easily be taken into account.

In our experiment [7] we measured the energies of the electrons ejected in forward direction from the process

$$He^0 + He \rightarrow He^+ + He^+ + e_1 + e_2. \quad (1)$$

In the simulation of the electron emission we assume that the final state of the collision is a correlated two-electron Wannier state centered at the outgoing projectile. Wannier threshold theories (e.g. [8]) predict that the electron pair angular correlation is characterized by the following Gaussian distribution

$$\frac{d^4\sigma}{dE_1' d\Omega_1' dE_2' d\Omega_2'} \sim \exp\left[-\frac{1}{2w^2}(\theta_{12}' - \pi)^2\right], \quad (2)$$

where $d^4\sigma/dE_1' d\Omega_1' dE_2' d\Omega_2'$ is the fourfold differential cross section (FDCS) for the two-electron emission differential in the electron energies E_1', E_2' and solid angles Ω_1', Ω_2'. w is the width of the Gaussian, θ_{12}' is the angle between the velocity vectors of the electrons. Primed quantities are used for the description of the electron emission in the projectile frame. According to Eq. (2) the Gaussian distribution has maximum at $\theta_{12}' = \pi$. The width of the distribution depends on the total energy, $E_t' = E_1' + E_2'$, it is a slowly increasing function of E_t':

$$\mathrm{FWHM} = 2\sqrt{2\ln 2}\,w = \alpha E_t'^{1/4}. \quad (3)$$

Here FWHM denotes the 'full width at half maximum' of the Gaussian, and α is a constant.

The simulation starts with a random creation of electron pairs in the projectile frame with 180° angular correlation. We assume that at the time moment when the simulation starts the collision fragments have already separated from each other to asymptotically large distances, i.e. they fly freely without any interaction between them. We assume, furthermore, that the electron pairs are emitted isotropically. We allow random deviations from the 180° correlation with the above Gaussian distribution. In Eq. (3) we apply $\alpha = 3.0$ (with E_t' given in atomic units). The latter value was obtained theoretically by Bartlett and Stelbovics [9] for electron-impact ionization of hydrogen, and was verified experimentally by Williams et al. [4].

For electron-impact ionization the total electron energy E_t' in Eq. (3) is the excess energy above the ionization threshold which is uniquely determined by the impact energy. In ion-atom collision E_t' has a continuous spectrum, its value depends on the amount of the transferred energy. We may assume that for small excitations above the threshold the cross section for the two-electron emission differential in E_t' can be expressed by a linear function:

$$\frac{d\sigma}{dE_t'} \sim c_0 + c_1 E_t'. \quad (4)$$

This approximation is justified by the fact that the energy of the electrons contributing to the cusp is very small in the projectile system. For 100 keV impact energy (collision velocity: 1 a.u.) the cusp is located at 13.6 eV. The whole energy range of the measurement in the laboratory frame is 8–20 eV. The corresponding energy range in the projectile frame is 0–1.5 eV, i.e. if we choose an energy value in this interval, its transformed value will be within the interval 8–20 eV. The coefficients c_0 and c_1 are free parameters of the model. In the experiment we measured relative cross sections, therefore only the ratio of the two coefficients has to be considered.

The electron energies E_1' and E_2' are obtained as follows. First we select the value of the total electron energy E_t' randomly with the distribution defined by Eq. (4). Then we share E_t' between the two electrons assuming *uniform* distribution. The 180° angular correlation given by Eqs. (2) and (3) and the uniform energy share are the most important predictions of the Wannier threshold theories (see, e.g. [8]). The latter prediction has been verified experimentally [10].

Using the obtained electron energies and emission angles, we determine the velocity vectors of the electrons. The energies E_1 and E_2 in the laboratory frame are calculated by Galilean transformation of the velocities. The conditions of the 'detection' of the electrons (observation and acceptance angles) are the same as they were in the real experiment: The entrance aperture of the two electron detectors had a rectangular shape defining acceptance (half) angles 0.5° and 1° in the two perpendicular directions. The detectors were located symmetrically with respect to the direction of the incoming beam at angles −0.5° and 0.5°. Other characteristics of the time-of-flight technique used for the measurement of the electron energies [11] (time resolution, finite projectile beam size, extended gas target) are also taken into account in the simulation.

3. Results and discussion

In Fig. 1 we present measured and calculated energy spectra of one of the electrons, e_1, ejected from the process (1) with the