Experimental investigation of the asymptotic momentum wave function of the He ground state

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Abstract. The correlated Kinematical Transfer Ionization channel cKTI in fast 4-body (p + He $\Rightarrow$ H° + He2+ + e) processes has been used to probe the highly correlated contributions to the asymptotic part of the He ground state wave function. In this reaction one electron with controlled initial momentum (2.5 to 7.5 a.u.) in the He ground state is kinematically captured by the proton at large impact parameters. The measured 3-particle final-state momentum distributions show features of a well-structured three-particle momentum wave function. We conclude that cKTI must almost exclusively proceed via the highly correlated and, virtually excited, non-s^2 contributions in the He ground state.

INTRODUCTION

Long-range correlation remains one of the most fundamental puzzles in the quantum mechanical world. Such correlations play a significant role in nature: they underlie much of the details in chemical bonding and prominent solid-state phenomena such as collective excitations (plasmons) and superconductivity. Furthermore, long-range correlation forces play a fundamental role in living matter, Bose-Einstein-Condensates (BEC) and halo nuclei [1]. Correlation in the asymptotic part of the atomic wave function plays a crucial role when atoms approach each other and may strongly influence the behavior of the atom in its chemical environment. Experimentally very little is known about this asymptotic part of the wave function, since direct measurements are rather difficult.

In atomic physics, the 3-particle wave function of ground state He provides the exemplary study of correlation in few-body systems [2]. It is one of the chemically least active atoms in nature and the non-s^2 part of the ground-state wave function is very small and is therefore difficult to probe with standard techniques such as spectroscopy. We will show that the high momentum components in the asymptotic part of the He ground state wave function contain significant non-s^2 contributions, both

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electrons necessarily composing an entangled $^1S_0$ state. In a Multi-Configuration Interaction (MCI) approach [3,4] these weak contributions are described by off-diagonal matrix elements (also called pseudo, off-shell, or virtually excited states) and together they are responsible for less than 10^{-6} of the total electronic density of the $^1S_0$ ground state. Nevertheless, these small fractions are of fundamental importance for the interaction of He with its environment [5] and [6]. It is to be stressed that while these non-s^2 asymptotic components are of less importance when it comes to the ground-state energy, the response of the ground-state He atom in certain reactions, as the one described below, proceeds only through the pathways of virtual states.

In this paper it is shown that the very weak non-s^2 components are essential for the correlated Kinematical Transfer Ionization (cKTI) process. This observation is unraveled by a novel multi-fragment coincidence technique. In the cKTI one considers the reaction p+He => H° + He^{2+} + e. The projectile proton is very fast with respect to the mean velocity of the bound electrons. One of the electrons of He is resonantly captured by the fast proton at relatively large distance from the He nucleus [7,8]. From the simultaneously measured transverse nuclear momentum exchange we have qualitative information on the nuclear impact parameter and select for our analysis only the very small H° deflection angles, i.e. distant collisions. Furthermore the initial velocity of the captured electron always exceeds the mean K shell velocity in He. We can conclude that the electron is captured in momentum space from the asymptotic part of the He ground state and as we discuss below very unlikely from regions close to the He nucleus.

In all cKTI processes, the He^{1+} recoil instantaneously fragments and the second electron is emitted into the H° scattering plane with a well-defined momentum vector. From the momentum vectors of the scattered H° and the recoiling He^{2+} target nucleus, we directly determine the correlated momentum wave function of both electrons in the asymptotic part of the initial ground state of He [8]. This method allows the measurement of the local parts of the asymptotic wave function (on the level of one part in 10^8 - 10^{10} of the total wave function) not observable by other techniques such as energy resolved spectroscopy of the ground state.

In the study presented here the cKTI transfer ionization channel [7,8] is chosen. Here, a fast proton captures at distant collisions (H° deflection angles below $5 \cdot 10^{-4}$ rad) one He electron (named number 1) nearly exclusively to the H° 1s state. The second electron (2) is simultaneously left in the continuum of He^+. In this channel the proton transfers a virtual photon and thus energy, but only a negligible amount of momentum to the He system. The perturbation of the correlated momentum wave function of He by the proton is rather small and can be neglected in comparison with the large initial momentum vectors of the two electrons. Since the force of the fast departing neutral H° on the remaining He^{1+} decreases rapidly, final-state interactions between the scattered projectile and the continuum fragments is negligibly small in this process.

The cKTI transfer ionization channel competes with other TI reaction channels [9, 10,11,12,13,14,15] where each channel leads to a characteristic location in the H° and He^{2+} final-state momentum phase space.

EXPERIMENT

To experimentally distinguish the different channels the recoil momenta and projectile momentum transfer have to be measured in coincidence with extremely high resolution (better than one part in 10^5 with respect to the projectile momentum). That is, the recoil ion longitudinal and transverse energy distribution have to be detected with 100 μeV resolution compared to, e.g., the 1 MeV proton impact energy E_p, to separate the cKTI channel from the other competing processes. There are 9 degrees of freedom in the final state and, thus momentum and energy conservation requires that 5 final state momentum components (3 of the He^{2+} recoil and the 2 H° transverse momentum components) are measured in coincidence. Further, very high detection efficiencies are needed as the cKTI cross section is typically only of the order of barns. Using the high momentum resolution and multi-coincidence efficiency of cold target recoil ion momentum spectroscopy (COLTRIMS) [16] the complete final-state momentum distributions for fast (400 to 1400keV) p + He => H° + He^{2+} + e transfer ionization processes (TI) were systematically measured at the 2.5 MV van de Graaf accelerator of the Institut für Kernphysik of the Universität Frankfurt. Details of the H° and He^{2+} coincidence experiment are given in reference [9]. The momentum resolution obtained is estimated to be < 0.3 a.u.

RESULTS AND DISCUSSION

For the cKTI process we can deduce from the measured final-state momentum distributions the initial-state momentum vector k_{e1} of electron 1. In Fig. 1 the pure

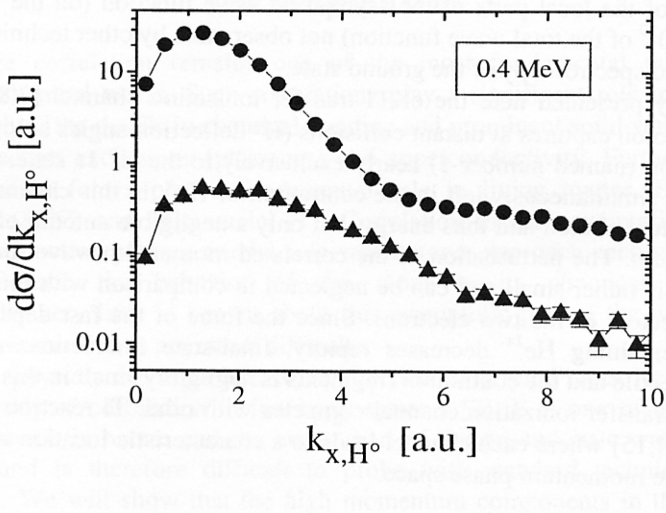

FIGURE 1. Singly differential pure capture (•) and TI (▲) cross sections as function of the H° transversal momentum $k_{x,H°}$ for 0.4 MeV proton impact energy.

single-electron capture and TI cross sections are shown as functions of the H° transversal momentum $k_{x,H^\circ} = m_p v_p \Theta_{H^\circ}$ at 0.4 MeV. At very small H° deflection angles Θ_{H° (region of peak structure) the proton is deflected only by the initial transverse momentum of the captured electron. Therefore the H° transverse momentum k_{x,H° is identical to the electron 1 transverse momentum in the initial state (measured with respect to the incoming projectile direction). Since for cKTI the initial-state velocity of electron 1 and that of the projectile must match (Brinkman-Cramer type capture), the complete initial-state momentum vector $\mathbf{k}_{e1} = (k_x, k_y, k_z)$ of electron 1 (where k_x is the transverse momentum component, k_y is the component perpendicular to the H° scattering plane and for each event is always set to zero, k_z is the longitudinal component) can be deduced from the measured H° transverse momentum with

$$\mathbf{k}_{e1} = (k_{x,H^\circ}, 0, \sqrt{(m_e v_p)^2 - (k_{x,H^\circ})^2}). \qquad (1)$$

The final-state momentum vector of electron 2 is deduced from the measured recoil momentum vector and the H° transverse momentum vector.

The surprising features of these measured correlated momentum patterns (see Fig. 2) are [7]:

1. The cKTI occurs only if the mean momenta of all 4 particles (the two electrons, the α nucleus, and the proton) are located in one plane.
2. The cKTI is most probable when electron (1), the recoiling He^{2+}, and electron (2) always share comparable momenta. In contrast, the cKTI process is unlikely if the momentum of these particles is peaked at zero.
3. Electron (2) is predominantly emitted into the backward direction.

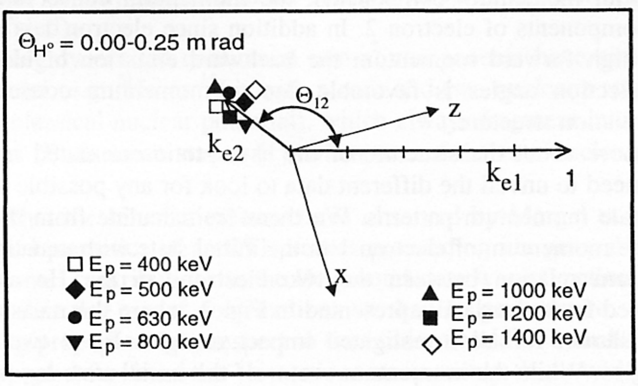

FIGURE 2. Initial state momentum relation between the two electron momenta $\mathbf{k}_{e1}$ and $\mathbf{k}_{e2}$ in He ground state derived from the data (see text) for different proton impact energies E_p. Momenta are scaled to $\mathbf{k}_{e1}=1$.

In [8] it is shown in detail that the present data are in full agreement with earlier, but less differential measurements [11] and that the experimental findings cannot be explained by any of the previously known TI channels or reaction mechanisms. Further, the observed final-state momentum pattern cannot be created by any uncorrelated scattering of three Coulomb particles fulfilling the energy, momentum and angular momentum conservation laws [8].

Concerning observation 1: As suggested in [8,9], 4-particle momenta in one plane are expected if in the cKTI process angular momentum is transferred from the initial He to the scattered H° (i.e. the cKTI process only occurs when the proton impact vector is parallel to the 3-particle momentum plane). Furthermore, as discussed in [8,9], at these high velocities the proton neither excites the electrons into a He and projectile p state (transfers to the electrons angular momentum) nor does it exchange angular momentum in the elastic collision with the He^{2+} nucleus. Thus, the angular momentum of the electrons in the final-state must reflect properties inherent in the initial He ground state as highly correlated, higher angular momentum components of both electrons in the $^1S_0$ ground state. According to Multi Configuration Interaction (MCI) calculations the global He ground state wave function contains about 1% non-s^2 contributions (mainly p^2 contributions) and each electron can indeed provide such angular momentum. Since for all cKTI events, He^{2+} and electron (2) mean momentum vectors are in the H° scattering plane, the cKTI process must proceed via the capture of non-s^2 electrons in the asymptotic region and the observed momentum patterns must reflect the initial angular momentum correlation of the non-s^2 contributions in the He ground state asymptotic wave function.

Concerning observation (2) and (3) above: the question is how can one explain the high shake-off energy of electron (2), sometimes above 200eV? Since electron (1) is captured from a non-s^2 component of the initial state electron 2 can never have zero velocity. Furthermore since the capture of electron 1 proceeds always via virtual states with high initial momentum components, the momentum conservation favors high momentum components of electron 2. In addition since electron 1 is mostly captured when it has high forward momentum the backward emission of electron 2 at very small H° deflection angles is favorable due to momentum conservation and the observed correlation structure.

To learn more about the structure of the asymptotic correlated momentum wave function, we need to unveil the different data to look for any possible scaling behavior in the final-state momentum patterns. We therefore calculate from the final state H° momentum the momentum of electron 1 in the initial state with equation 1. The initial state momentum relation between the two electrons in the He asymptotic wave function derived from the data is presented in Fig. 2, where the measured momentum relations are shown for all investigated impact energies E_p at two very small H° scattering angles. While the momentum vector of the initial state $\mathbf{k}_{e1}$ is always plotted to the right and normalized to 1, the momentum vector $\mathbf{k}_{e2}$ is scaled in its length too for all ten different energies of the projectile E_p. The sign of the angle between the electrons Θ_{12} is defined by the H° deflection, – sign being opposite to the H° deflection. The z direction is defined by the incoming projectile and the x direction by the H° transverse deflection. For all systems investigated the relative angle between electron 1 and 2 appears nearly constant with Θ_{12} = -140° +/- 15°. Also the ratios of the magnitudes of the momenta are constant within the experimental uncertainty of about 20%. It is striking to see that the cKTI process always yields a discrete momentum pattern.

The asymmetry of the momentum pattern in the final state (seen from above the plane in a clockwise direction) is striking. We find that electron 2 is always emitted opposite to the proton. This directional asymmetry points to the important role of high angular momentum components of the He wave function. Classically we can consider that electron (1) is captured by the proton when it is generally closer to the proton than to the α nucleus and r_{e1} (the electron (1) position vector relative to the α nucleus) always points in the positive x direction. Furthermore the captured electron (1) has to move forward, i.e. in the positive z direction. This means that the orientation of the electron angular momentum, i.e. its m-value, always points upward with respect to the H° scattering plane. Since electron (2) must have exactly the opposite angular momentum, its angular momentum is also oriented with m= -1 (for p^2 components).

So far all theoretical attempts to explain these structures have failed completely. The theoretical studies of Popov et al. [18] demonstrate that correlated helium wave functions better reproduce the single differential cross sections both for TI and SC reactions, especially for large projectile energies, but many details (absolute values and angular position of maxima) were not well described. This can be understood in the following way. The authors used trial variational helium wave functions, which concentrated on the space domain out to 0.6 a.u. and did not include contributions of highly excited (continuum) states, which we observe. For projectile energies $E_p > 1$ MeV the impact parameter becomes comparable to the mean helium radius, and variational wave functions give better and better results. But these functions are not able to describe properly the asymptotic space domain important at smaller projectile energies. Recently Popov and Ancarani showed [17] that the asymptotic behavior of all "traditional" helium ground state wave functions is not correct, and the mutual angle of the bound helium electrons in the space asymptotic domain is an integral of motion (i.e. it is fixed).

These virtual highly excited continuum non-s^2 components have similarities with halo states in nuclei (e.g. ^{6}He or ^{11}Li, with a core and two nucleons rotating at large radii outside the classical nuclear potential), which always fragment into the core plus two free nucleons (Borromean states) [1], when one of the two nucleons is knocked off.

We conclude that the kinematical structures observed by Mergel et al. [7] can be interpreted by the kinematics of a cKTI process proceeding via generalized shake-off processes from non-s^2 contributions in the He ground state wave function. Furthermore we have shown that the non-s^2 contributions in the He groundstate wave function contain interesting properties with respect to the hidden world of correlation. The very fast electrons captured far from the He nucleus are possibly those with the strongest dynamical e-e-correlations. As shown in [8] the relative contribution of non-s^2 components increases with increasing momentum since the cKTI process becomes relatively more important with increasing proton energy.

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