Vortices associated with the wavefunction of a single electron emitted in slow ion-atom collisions

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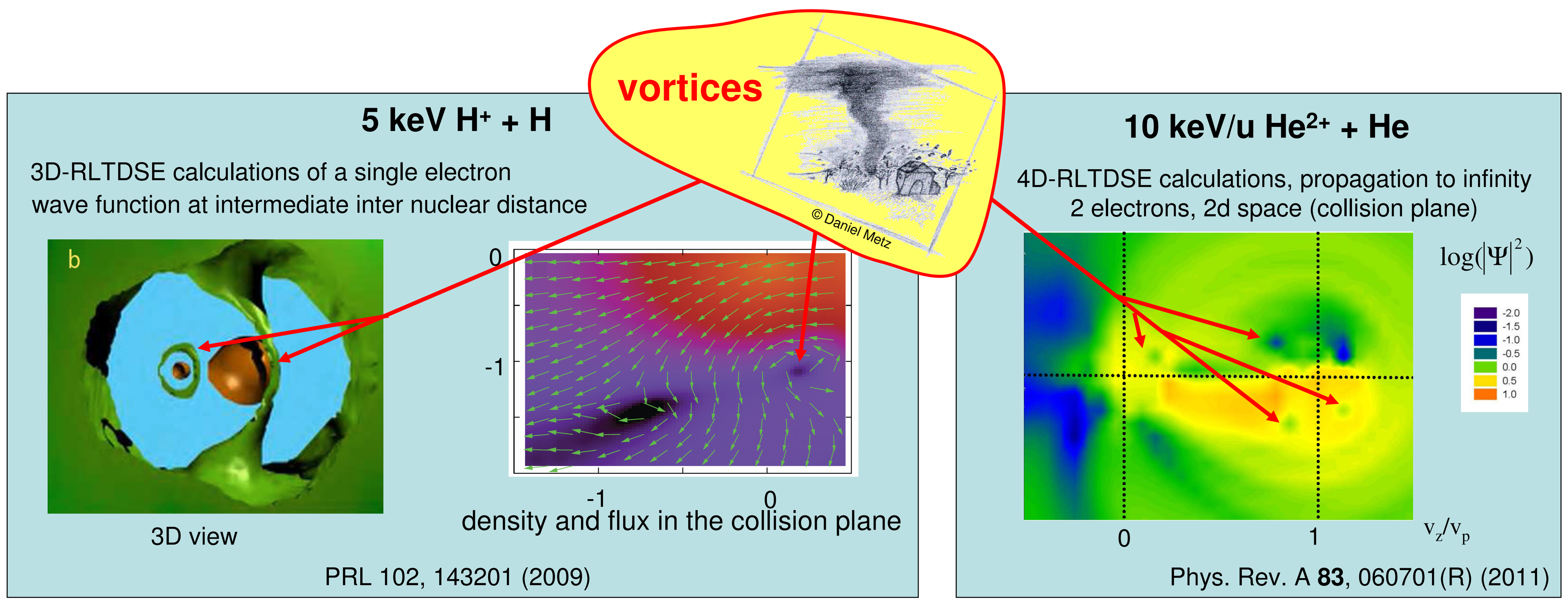
Using COLTRIMS we measured the momentum distribution of electrons emitted during slow ion-atom collisions 10 keV/u He^{2+} + He → He^{+} + He^{2+} + e^-. At large scattering angles above 2 mrad it shows rich structures, which have not been observed in earlier experiments. They arise from two-electron states absent in an independent electron picture of the transfer ionization process. Our calculations reveal that minima in the measured distributions are zeroes in the electronic probability density resulting from vortices in the electronic current.

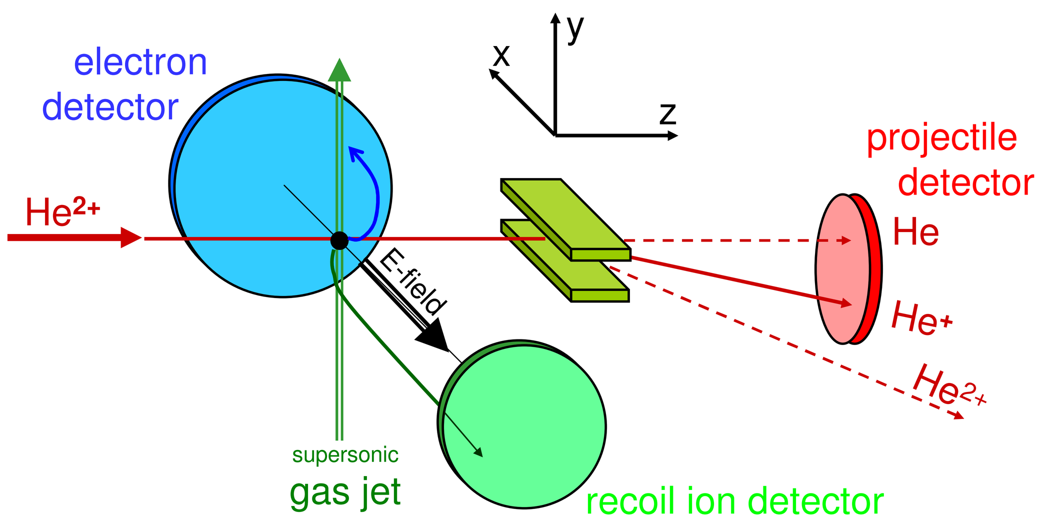
Motivation:

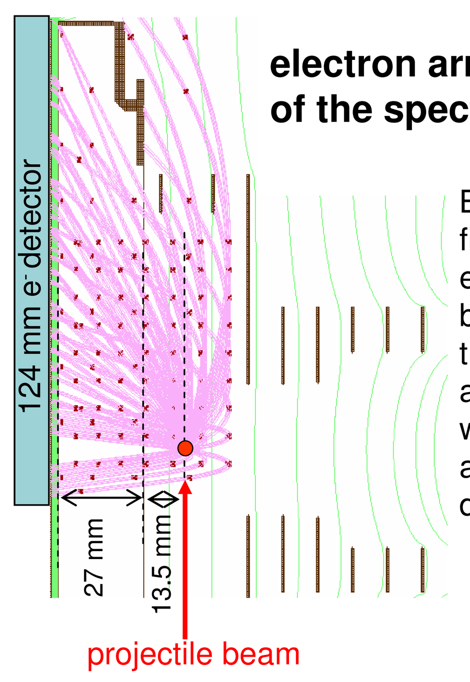
The time depended Schrödinger equation of a single electron at the potential of two nucleus moving at a classical trajectory can be solved at a regularized lattice of 3 dimensions (3D-RLTDSE). The free electron wave function shows vortices which are lines with zero probability density surrounded by a flux. Because of limited computing power, 2 electron systems have only be treated in the collision plane (2D space) which still requires a 4D lattice. However, vortices have been predicted to appear in the reaction He^{2+} + He ➔ He^{+} + He^{2+} + e- at an impact velocity of 0.63 a.u. (10 keV/u) and 1 a.u. impact parameter. We tried to prove this experimentally.



Experimental setup:

COLTRIMS with low electric field and without magnetic field

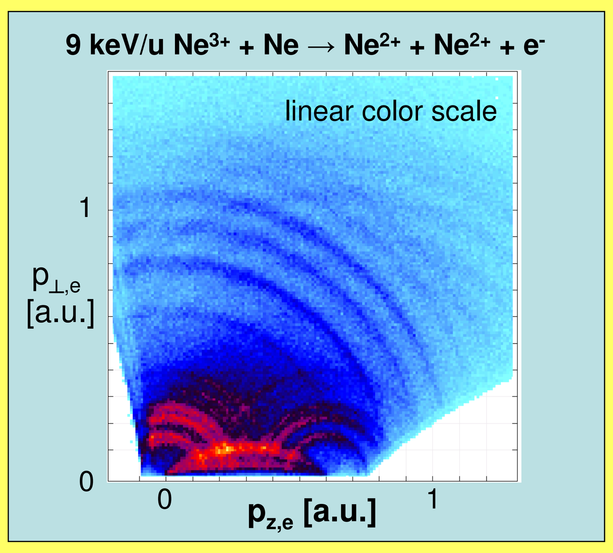




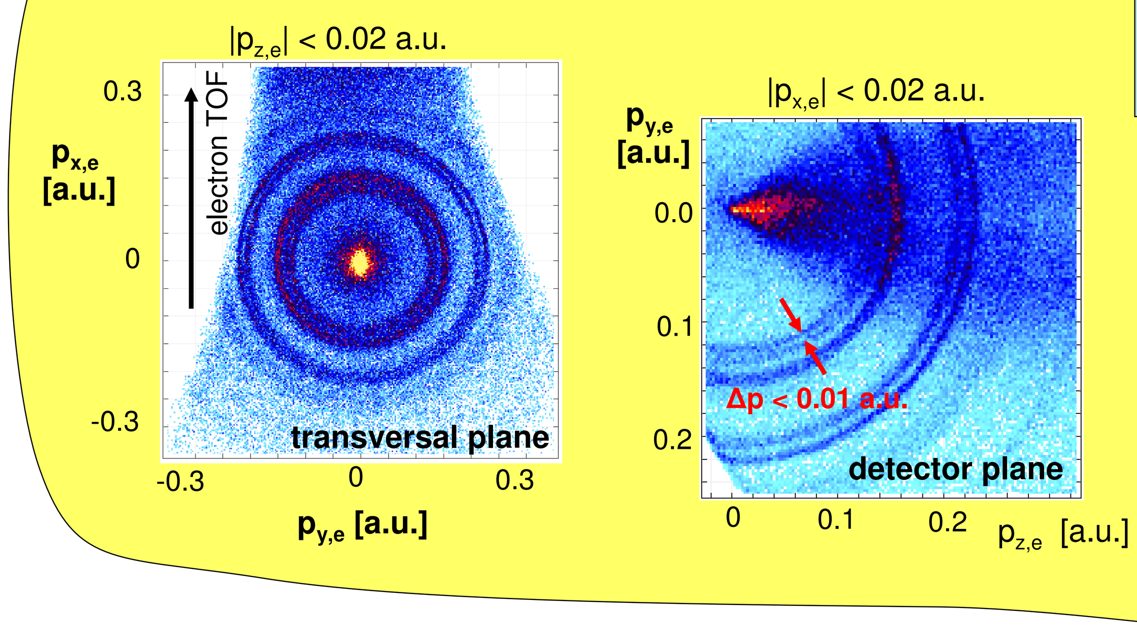
electron arm of the spectrometer:

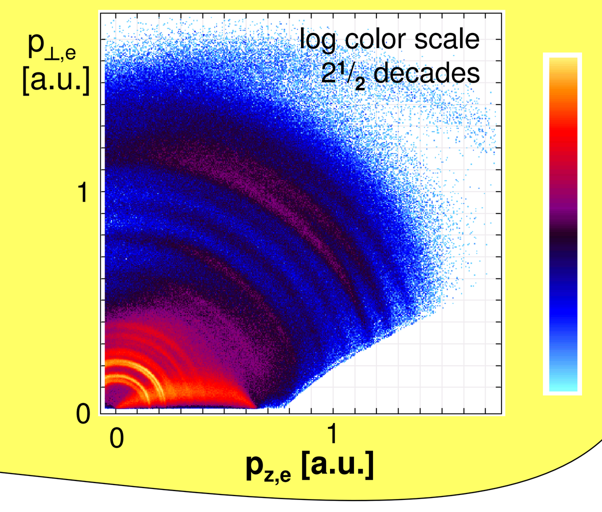
By applying a low electric field of about 1 V/cm electrons with velocities between the target and the projectile ion are spread over the whole active surface of an Ø 124 mm MCP detector

The electron spectrometer can be tested and calibrated by measuring low energetic **electrons emitted from auto ionizing states of Ne^{+}.**

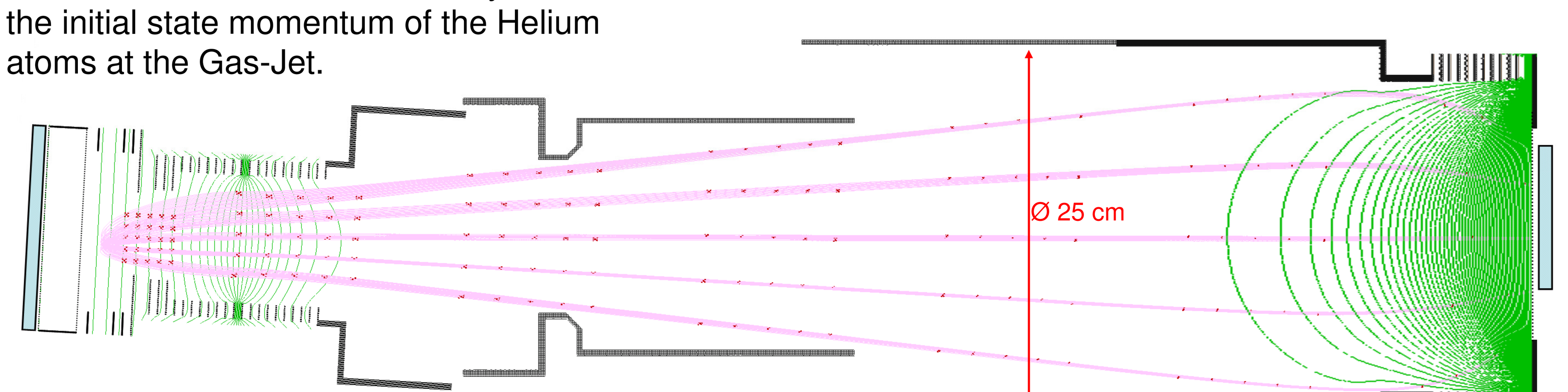


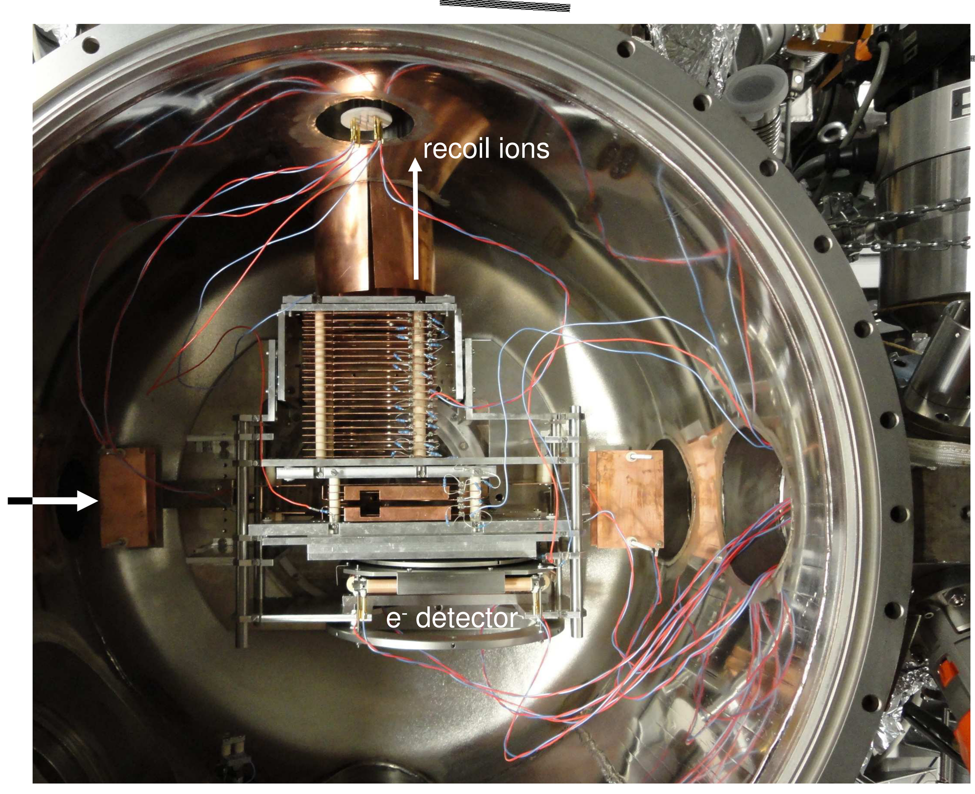
10 keV/u He^{2+} + Ne → He^{+} + Ne^{2+} + e^-





Recoil ion trajectory simulation in the transversal plane
The momentum distribution is asymmetric because of the initial state momentum of the Helium atoms at the Gas-Jet.

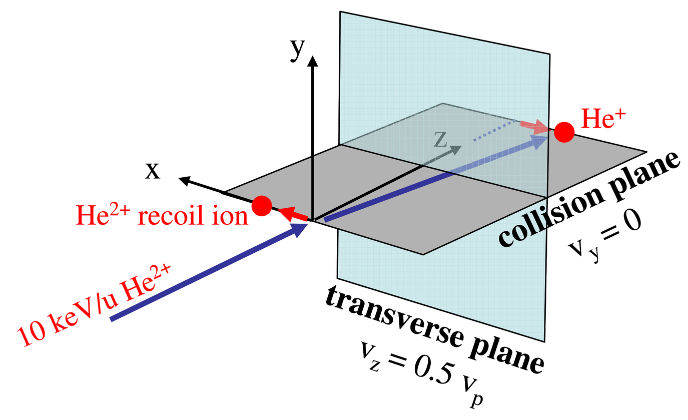




Results:

Emitted electron velocity distributions are presented in a coordinate frame defined by the nuclear motion (shown right).
We use only those reactions where the bound electron is in the ground state of the outgoing He^{+} projectile.

Because the direct measurement of the projectile scattering angle had a rather poor resolution we calculated the scattering angle from the measured momenta of the electron and the recoil ion.



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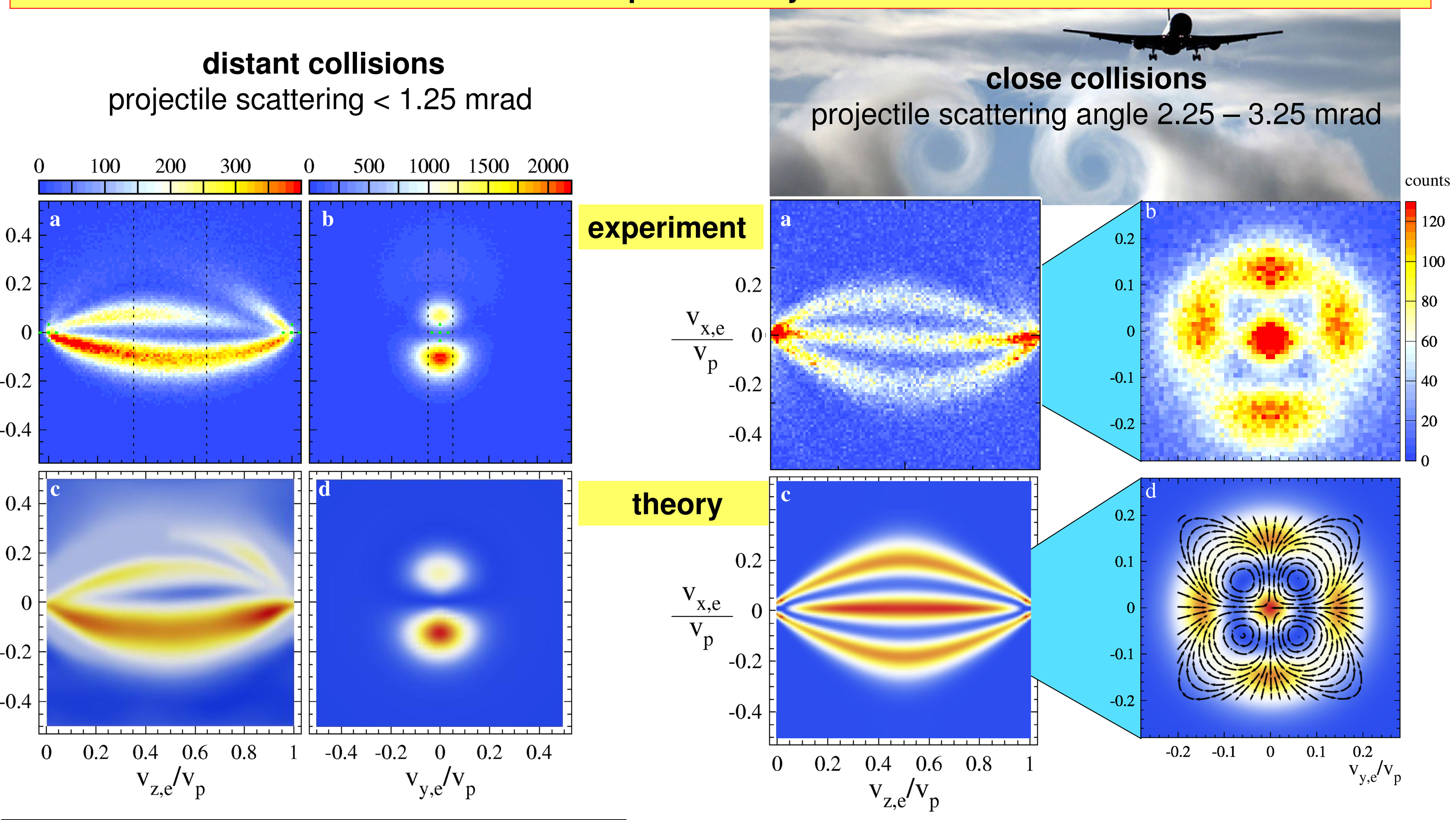
At **distant collisions** we observed the well known "two bananas" structure, which can be explained by the promotion of the $2p\pi_u$ quasi-molecular state to the continuum. Because of the improved resolution and statistics a third banana became visible but **experimentally vortices have not been observed.**



The 4D-RLTDSE calculation which motivated the measurement has several problems:

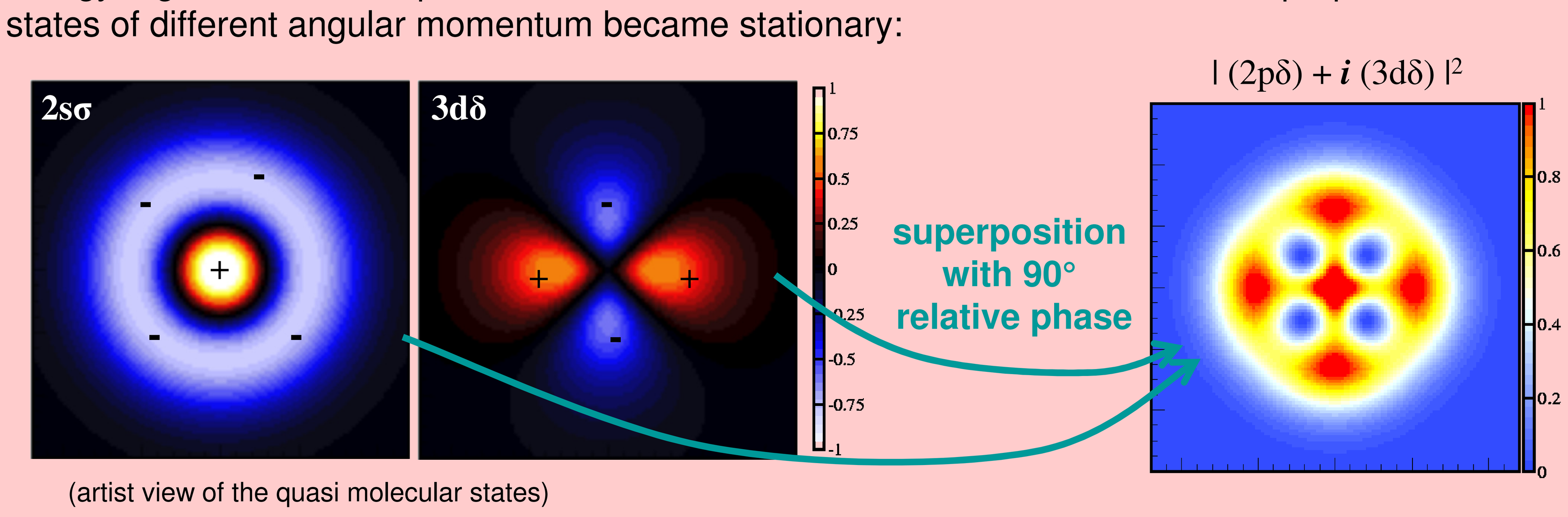
- limitations to 2D
- insufficient representation of the bound electron at the end of the propagation because of the scaling of the grid to the internuclear distance
- calculation for a specific impact parameter, no coherent superposition of different nuclear trajectories contributing to the same scattering angle

Our coworkers from Texas and Tennessee developed a new theoretical approach named 2eHC-RLTDSE:

- **Hidden crossing** promotion of quasi-molecular states using fully correlated Sturmian type two electron wave functions of the He_2^{2+} quasi molecule. Calculation of the amplitude of states as a function of the impact parameter at intermediate internuclear distances (about 10 a.u.)
- Calculation of the amplitudes as a function of the momentum transfer by 2D-Fourier transformation.
- Projection to a new basis of product states of a bound and a nearly ionized electron
- **3D-Regularized Lattice propagation** (RLTDSE) of only that electron which gets ionized using screened nuclear potentials.

Appearance of free vortices at the transversal plane:

By the propagation of the emitted electron wave function to infinite internuclear distances the energy Eigen value of all quasi molecular states convert to zero. Therefore the superposition of states of different angular momentum became stationary:



(artist view of the quasi molecular states)

To create the vortices, the 3dδ quasi-molecular state has to be populated, which is not efficiently done by dynamical couplings between states of a single active electron. At the He_2^{2+} quasi-molecule an angular momentum of 2ħ can be given to the emitted electron at the crossing between (1sσ,3dδ) and the initially populated state $(2p\pi)^2$: The emitted electron gets the angular momentum of both electrons.

The relevant states cross at about 0.9 a.u. internuclear distance, therefore close collisions are needed to create the vortices.

He^{2+} + He(1s²) → He^{+}(1s) + He^{2+} + e^- at other **impact velocities v_p and scattering angles:**