# Magnetic Manipulation of Rotational Orientation Projection States in Ground State Molecules

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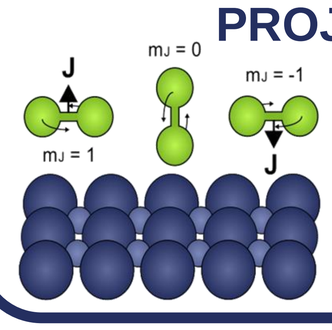
European Research Council
Established by the European Commission

Supported by Horizon 2020 Research and Innovation Programme Grant Number 772228

## INTRODUCTION

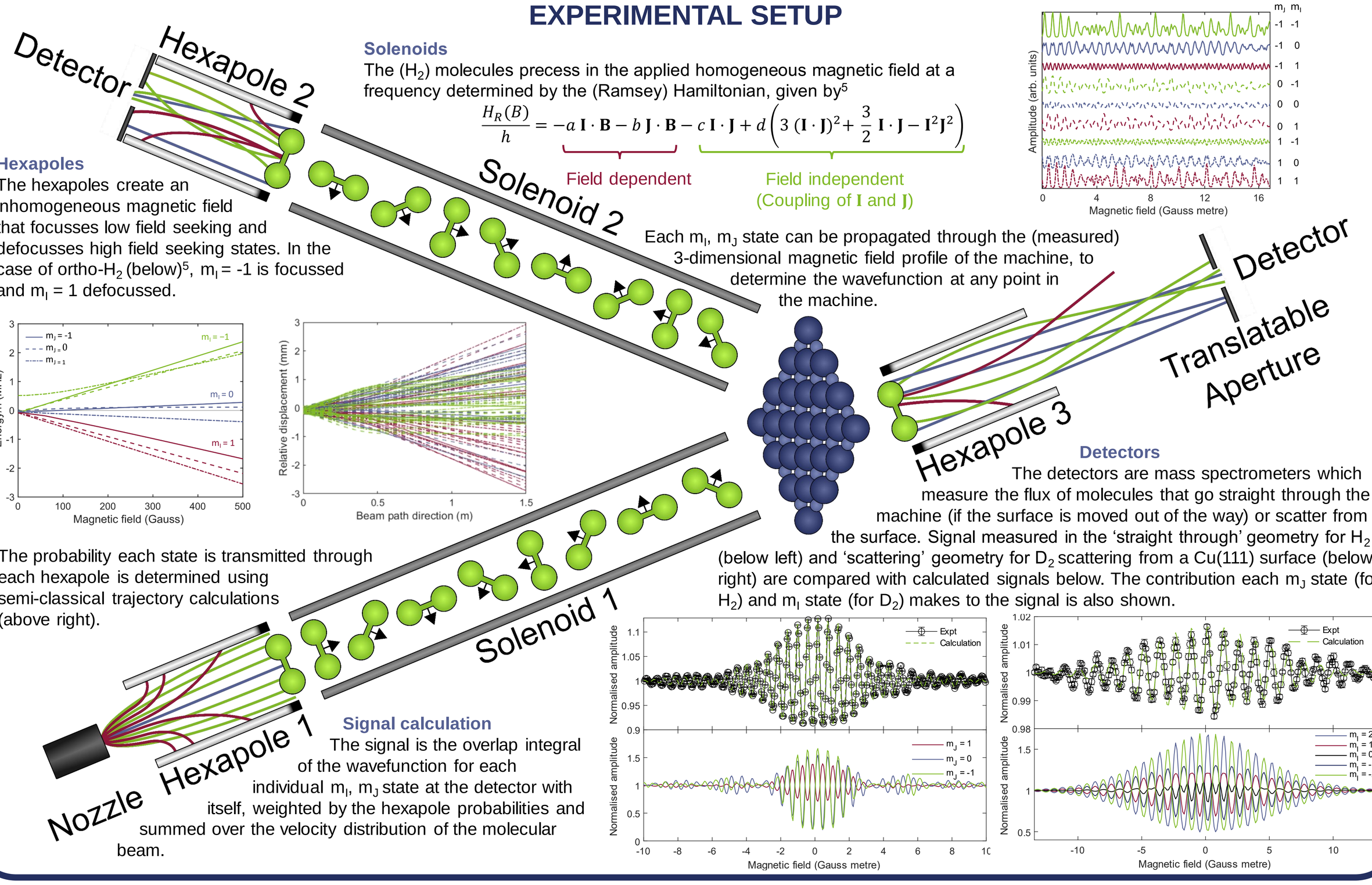
Creating spatially anisotropic samples of gas phase molecules to study steric effects in gas-surface collisions has been typically limited to those that can be prepared by laser excitation[1] or to paramagnetic molecules[2]. Here we present a recently developed technique[3] which can be used to prepare and manipulate the rotational orientation and nuclear spin projection states of ground-state molecules. We will also show a summary of the results from the first application, the extraction of a scattering matrix for $H_2$ scattering from LiF(100)[4]. These results will provide extremely stringent benchmarks which will help develop and benchmark accurate theoretical models.

## ROTATIONAL ORIENTATION PROJECTION STATES




Rotational orientation projection states define (classically) whether a molecule is rotating like a helicopter or cartwheel. The nuclear spin (**I**) projection states define the projection of **I** ($m_I$) onto the same quantisation axis.

## EXPERIMENTAL SETUP




### Solenoids

The ($H_2$) molecules precess in the applied homogeneous magnetic field at a frequency determined by the (Ramsey) Hamiltonian, given by[5]

$$\frac{H_R(B)}{h} = \underbrace{-a\,\mathbf{I}\cdot\mathbf{B} - b\,\mathbf{J}\cdot\mathbf{B}}_{\text{Field dependent}} \underbrace{- c\,\mathbf{I}\cdot\mathbf{J} + d\left(3\,(\mathbf{I}\cdot\mathbf{J})^2 + \frac{3}{2}\,\mathbf{I}\cdot\mathbf{J} - \mathbf{I}^2\mathbf{J}^2\right)}_{\text{Field independent (Coupling of I and J)}}$$




### Hexapoles

The hexapoles create an inhomogeneous magnetic field that focusses low field seeking and defocusses high field seeking states. In the case of ortho-$H_2$ (below)[5], $m_I$ = -1 is focussed and $m_I$ = 1 defocussed.







The probability each state is transmitted through each hexapole is determined using semi-classical trajectory calculations (above right).

Each $m_I$, $m_J$ state can be propagated through the (measured) 3-dimensional magnetic field profile of the machine, to determine the wavefunction at any point in the machine.

### Detectors

The detectors are mass spectrometers which measure the flux of molecules that go straight through the machine (if the surface is moved out of the way) or scatter from the surface. Signal measured in the 'straight through' geometry for $H_2$ (below left) and 'scattering' geometry for $D_2$ scattering from a Cu(111) surface (below right) are compared with calculated signals below. The contribution each $m_J$ state (for $H_2$) and $m_I$ state (for $D_2$) makes to the signal is also shown.





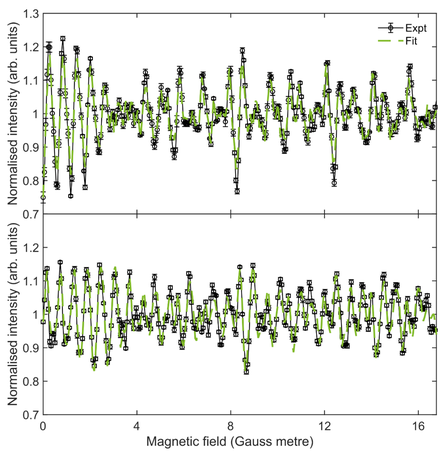


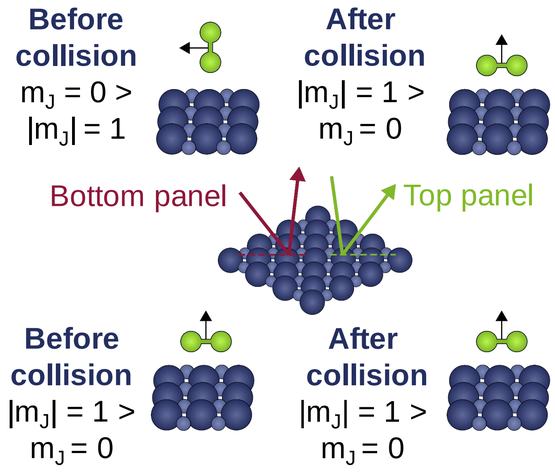
### Signal calculation

The signal is the overlap integral of the wavefunction for each individual $m_I$, $m_J$ state at the detector with itself, weighted by the hexapole probabilities and summed over the velocity distribution of the molecular beam.

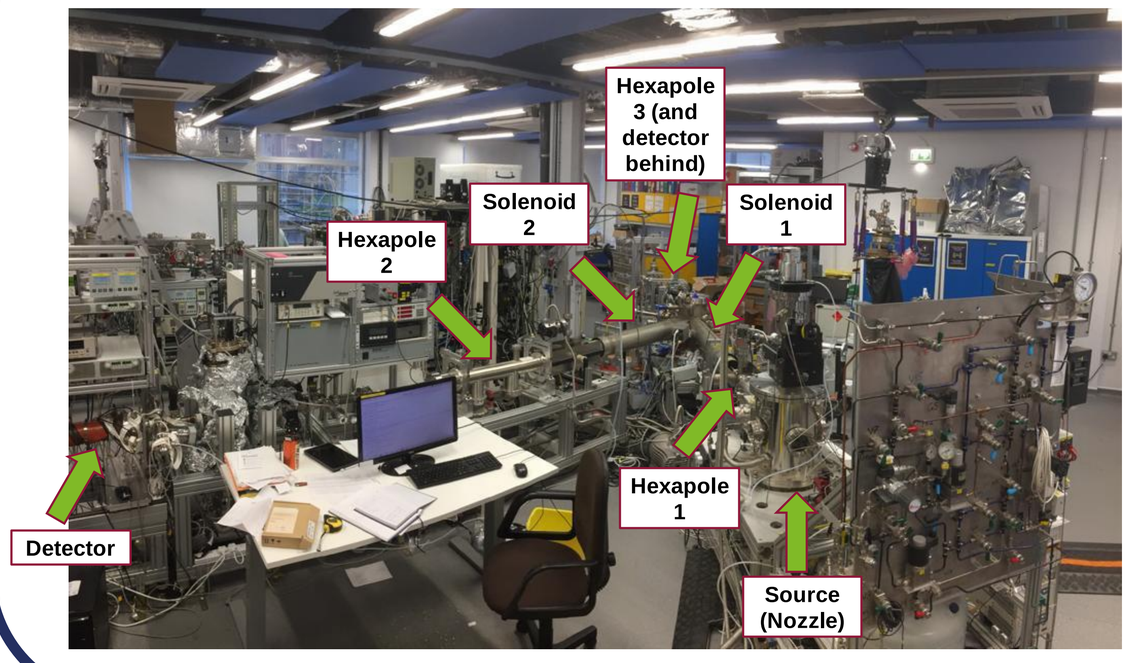
## DETERMINING A SCATTERING MATRIX $H_2$ SCATTERING FROM LiF(100)[4]

The scattering matrix characterises how the wavefunction changes when the molecules scatter from the surface. The different elements give information about the rotational orientation states that scatter into and from the surface in different directions.




## THE MACHINE

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