

The peak shape of electrons scattered ‘elastically’ from H₂ not a delta function or a Gaussian but almost a cusp

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Synopsis The intrinsic energy distribution of keV electrons scattered ‘elastically’ from H₂ over large angles is measured and compared to calculations. It is neither a delta function or a Gaussian but has, in particular at low temperatures, an almost cusp-like shape that reflects the linear nature of the H₂ molecule.

The elastic peak observed in an electron scattering experiment is often considered to have a shape that is just a fingerprint of the spectrometer performance. For scattering of keV electrons over large angles this is not true and the peak shape contains information about the scattering molecule. Here we demonstrate that the linear nature of the H₂ molecule is reflected in the peak shape.

When a keV electron is scattered over large angles there is a size-able momentum transfer \mathbf{q} . The scattering target, assumed initially at rest, will acquire this momentum and hence a kinetic energy $q^2/2M$. What is the appropriate choice of M for H₂: the mass of the H₂ molecule or the H Atom? Experimentally it turns out to be the latter, i.e. the electron scatters incoherently from a single atom [1].

The second observation is that the elastic peak for H₂ is much broader than the experimental resolution. The H atom is moving and hence Doppler broadening affects the energy transfer in the e⁻-H collision. Especially at low temperatures the motion is dominated by the zero-point vibrational motion of H₂. As the potential is close to harmonic, the H momentum distribution is Gaussian. The width of the peak reflects thus the kinetic energy of the scattering atom. Initially it was assumed that the observed peak shape could be described by a Gaussian. The obtained fit was not perfect and the inferred kinetic energy was systematically smaller than the calculated one [2].

More precise measurements taken with a gas cell, where the H₂ molecules is in thermal equilibrium confirmed these observations initially made using hydrogen effusing from a needle in a cross-beam configuration [3].

It turns out that the Doppler broadening can not be described by a Gaussian. This is understood by considering how the line-shape varies with the angle between the molecular axis I and \mathbf{q} . If \mathbf{q} is perpendicular to I then the Doppler broadening due to the vibrational motion is absent. The broadening is maximum for I along \mathbf{q} . The experimental line shape is the sum of the contribution of all orientations and turns out to have (at 0K) a cusp shape. In the exper-

iment, done at 120°K, the cusp shape is somewhat washed out due to the contribution of Doppler broadening due to translations and rotations, but deviations from Gaussian are still evident. Analysing the experiment with the proper lineshape gives a mean kinetic energy close to the calculated one [3].

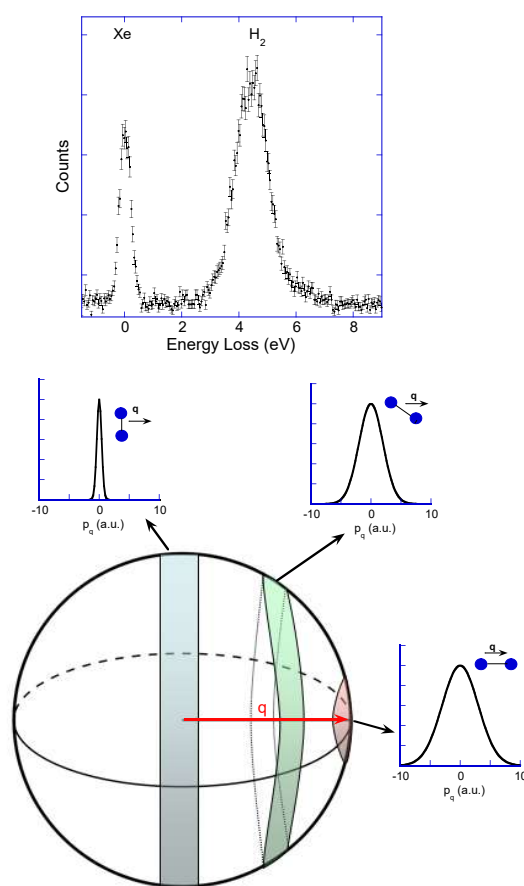


Figure 1. The top graph shows the spectrum of a Xe-H₂ mixture measured at 4keV and a scattering angle of 90°. The lower half shows the effect of the molecular orientation to its contribution of the spectrum

References

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