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Mass-selective spectroscopy of nuclear momentum distributions: ionic compounds and beyond

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Neutron Compton scattering (NCS) is a unique experimental technique made possible by the development of epithermal neutron sources, such as the ISIS source of the Rutherford Appleton Laboratory in the UK. The measurement of nuclear momenta by high-energy neutron Compton scattering relies on the fact that the energy and momentum transferred in the scattering process are sufficiently large, such that the so-called impulse approximation (IA) is an accurate starting point. In the IA limit, the dynamic structure factor measured in NCS for a given nucleus covers the whole energy range of its motional modes. This includes translational and rotational modes, followed by lattice and internal molecular vibrations.

Since its birth, the NCS technique has been employed to study proton momentum distributions in quantum fluids and solids, metal hydrides and gas and charge-storage media, etc. Beyond the proton, recent instrument developments other the prospects of access to the NMDs of heavier nuclides including deuterium, helium, lithium, carbon, oxygen, and fluorine.

The work presented here seeks to fill the gap in the methodology of the determination of nuclear momentum distributions using epithermal neutrons by providing two specific examples of a direct and simultaneous access to the momentum distributions and mean kinetic energies of lightweight and heavy nuclei in two systems: (i) an ionic compound – lithium hydride and its deuterated counterpart, and (ii) squaric acid – an above room temperature organic antiferroelectric. It is demonstrated that, beyond the usual case of proton, the determination of the shapes of momentum distributions of heavier nuclei, deuterons and lithium, is also possible. Moreover, the work demonstrates that, in case of oxygen and carbon, also kinetic energies can obtained directly from neutron Compton scattering experiments. On the scientific front, the presented data provide stringent benchmarks for first-principles calculations on these technologically relevant materials. From an instrumentation point of view, the presented experiments serve as preliminary assessment of current capabilities of mass-selective nuclear momentum distribution measurements (MANSE) of heavy nuclei using the electron-volt spectrometer VESUVIO at ISIS.

Keywords: Neutron Compton scattering; nuclear momentum distribution; ionic compounds; organic antiferroelectric compounds.