“Progress in Electron Volt Neutron Spectroscopy” workshop

Abstracts

Author: J Mayers, Rutherford Appleton Laboratory, Chilton, Didcot,OX110QX, UK.

Title: The VESUVIO spectrometer

Abstract:

The inverse geometry spectrometer VESUVIO operating on the ISIS pulsed neutron source has pioneered Deep Inelastic Neutron Scattering measurements of the momentum distribution of light atoms in condensed matter systems. These measurements provide a probe of the local structure of the materials as well as information on the dynamics of the atoms. We provide here a summary of the progress made to date in instrument development, data analysis and the interpretation of the results, for a variety of physical systems chosen to illustrate the scope and power of the method. These include measurements on the quantum fluids ^{4}He, ^{3}He, ^{3}He-^{4}He mixtures, liquid and solid neon and hydrogen containing systems such as metal hydrides and hydrogen bonded liquids and solids.

Author: R. Senesi, Università degli Studi di Roma Tor Vergata, Dipartimento di Fisica, via della Ric. Scientifica 1, 00133 Roma

Title: Momentum distribution in quantum systems

Abstract:
Liquid 3He, 4He and 3He-4He mixtures represent prototype quantum liquids formed of fermions, bosons and mixed fermions-bosons. The momentum distribution n(p), and its second moment, the atomic mean kinetic energy <Ek>, are fundamental quantities for the microscopic description of these systems. Inelastic Neutron Scattering at high momentum transfer is the most relevant experimental technique for the determination of n(p) and <Ek>. Recent measurements carried out at the ISIS spallation neutron source are reported and compared with advanced quantum Monte Carlo simulation results.

Author: G. F. Reiter, Physics Department, University of Houston, Houston, Texas

Title: Imaging of interatomic Born-Oppenheimer potentials

Abstract:
Deep Inelastic Neutron Scattering measures the tomographic projection of the 3-D momentum distribution of the target particle, and can be inverted to give the momentum distribution n(p). In the case that the particle sits at a center of inversion symmetry, is sufficiently isolated from other light particles that a one-particle interpretation is valid, and the temperature is sufficiently low that the particle can be considered to be in the ground state of its potential well, n(p) can be used to

calculate the shape of the potential in which the light particle is confined. We apply this procedure to the first fully 3-D direct measurements of the Born-Oppenheimer potential for a proton in any system. In particular, we do this for the hydrogen bonded system Rb3H(SO4)2 at 10K and 70K. The potential along the bond is found to be a single well, with a barrier to moving to an adjacent well of 400mev. The method is suffiicently sensitive to detect the changes due to thermal expansion.
Comparison with earlier phenomenological models of the hydrogen bond using double Morse potentials show that these are in semi-quantitative agreement with the measured results

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Title: Proton momentum distribution of water up to Critical Point and confined in xerogel.

Abstract:
Studies of single-particle momentum distributions in light atoms and molecules are reviewed with specific emphasis one experimental measurements using the deep inelastic neutron scattering (DINS) technique at eV energies.The remarkable development of these technique will be reviewed. These types of measurements provide a unique probe of the short-time dynamics of the recoiling atoms or molecules as well as information on the locals tructure of the materials. The theoretical framework for the interpretation of DINS experiments will be introduced and the physical principles underlying the impulse approximation from light atoms and molecules thoroughly illustrated. The experimental technique is critically presented and it will be shown how, in some cases, these measurements can be used to extract directly the effective Born–Oppenheimer potential. Most recent results from experimental studies performed on a water in sub- and super-critical condition in bulk and confined geometry will be discussed

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Title: Single proton dynamics of water in carbon nanotubes

Abstract:
The incorporation of water into carbon nanotubes provides a simple analogue of biologically important trans-membrane channels and so is of large interdisciplinary scientific interest. Recently [1] we have studied quasi-one-dimensional water encapsulated inside single wall carbon nanotubes (SWNT) of 14 Å diameter (and ~10 μm long), here referred to as *nanotube-water*, by means of neutron diffraction, inelastic and quasielastic neutron scattering in parallel with MD simulations (performed using the TTM2-F polarizable flexible water model with smeared charges and dipoles). The observed extremely soft dynamics of nanotube-water at low temperatures were consistent with the MD model that includes shell water molecules near the inner wall of the nanotubes plus central water-chain structure. It was found that these chain water molecules are responsible for the observed large mean square displacements which are a result of their low coordination and weak bonding to the outer shell. Here we extend this research for water confined in SWNT of different diameters, at different pressures and temperatures. Using a ‘parallel tempering’ MD algorithm, we were able to calculate the structural and dynamical properties of nanotube-water from low to high

temperatures, which clearly showed the phase transition on heating from high to low density liquid at ~200 K. Above the phase transition the structure becomes a disordered H-bonded network similar to the bulk liquid. Applying a high pressure results in decreasing the mean-square displacement of nanotube-water at low temperatures, comparable to that in bulk ice. The measured vibrational density of states of nanotube-water at P=3.7 kbar shows features similar to that for high-density amorphous (hda) ice. MD simulations for nanotube-water under pressure describe well the observed phenomena and show large change in its structure: water becomes more dense (by ~30%) like a bulk ice. Deep inelastic neutron scattering (DINS) shows that at low temperature the momentum distribution for nanotube-water protons is much narrower compared to other forms of bulk water (ice-Ih, hda-ice and ice- VI), reflecting their large spatial delocalization [2]. At temperatures above 230 K and also under pressure (3.7 kbar) at 40 K the measured momentum distribution broadens to the values similar to bulk water/ice. The kinetic energy for ground-state nanotube-water protons at 5 K is about 30% smaller compared to other ice forms. Thus, DINS clearly shows that the quantum state of the nanotube-water in the low temperature phase is qualitatively different from that of any phase of water seen so far, and the possible explanation will be discussed.

[1] A.I. Kolesnikov *et al.*, *Phys. Rev. Lett.* **93**, 035503 (2004).
[2] G. Reiter *et al., Phys. Rev. Lett.* (2006) in print.

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Title: Intensity deficit in DINS from protons – Attosecond Schrodinger-Cat states

Abstract:
Several neutron Compton scattering (NCS, also called DINS) experiments [1,2] on liquid and solid samples containing protons or deuterons show a striking anomaly, which is a shortfall in the intensity of epithermal neutrons scattered by the protons and deuterons. E.g., neutrons colliding with water for just 100-500 attoseconds (1 as = 10^{-18} s) will see a ratio of hydrogen to oxygen of roughly 1.5 to 1, instead of 2 to 1 corresponding to the chemical formula H_2O. The experiments were done at the ISIS neutron spallation facility,UK. Due to the large energy and momentum transfers applied, the duration of a neutron-proton scattering event is a fraction of a femtosecond which is extremely short compared to condensed-matter relaxation times.
Recently this effect has been confirmed [2] using an independent method, electron-proton Compton scattering (ECS), at the Australian National University. ECS experiments from a solid polymer showed the exact same shortfall in scattered electrons (with energy about 20-35 keV) from hydrogen nuclei, comparable to the shortfall of scattered neutrons in accompanying NCS experiments on the same polymer. The similarity of the results is striking because the two projectiles interact with protons via fundamentally different forces – electromagnetic and strong.
Theoretical considerations suggest the presence of short-lived quantum entanglement of the scattering protons and the surrounding electrons, so that the usual Born-Oppenheimer approximation is not applicable. The relevant physical frame for the theoretical treatment of the considered effect may be given by the quantum dynamics of open quantum systems, cf. [3].
Further experiments applying related scattering methods with much higher energy transfers (and scattering times about 1 as) are under consideration.

[1] C. A. Chatzidimitriou-Dreismann et al., Phys. Rev. Lett. **79**, 2839 (1997)
[2] C. A. Chatzidimitriou-Dreismann et al., Phys. Rev. Lett. **91,** 057403 (2003)
[3] C. A. Chatzidimitriou-Dreismann, Laser Physics 15, 780 (2005)

Author: C. D. Frost, ISIS Facility, CCLRC Rutherford Appleton Laboratory, Chilton, OXON, OX11 0QX, UK

Title: Soft Errors investigations with MeV neutrons

Abstract:
The generation of soft-errors in electronics from atmospheric fast neutrons that are produced by cosmic radiation has been increasingly investigated over the last few years within the avionics industry. More recently the sensitivity of ground based electronics to atmospheric fast neutrons has also become of increasing concern as these increasingly complex devices are uses in a huge array of applications, including mission and safety critical systems. Accelerated testing of electronic components in a neutron radiation flux that mimics these atmospheric neutrons has therefore become strategically important to both the avionic and other sections of the electronics industry. Here the recent development of a test facility for fast neutron effects on electronic systems on the VESUVIO beam-line at the ISIS Facility will be reported.

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Title: The Very Low Angle Detector on VESUVIO

Abstract:

VESUVIO is an inverted geometry time-of-flight neutron spectrometer originally designed for momentum distribution investigations of light nuclei in condensed matter by the application of the Deep Inelastic Neutron Scattering (DINS) technique. In the DINS regime high energy transfers, >1eV, and high momentum transfers, >20 $Å^{-1}$, are required. The experimental setup of VESUVIO underwent a major upgrade within the EU funded project, eVERDI. The latter project included, among other items, the installation of the VLAD bank, covering the angular range of $1^{\circ}<2\theta<5^{\circ}$. This allows to exploit the High-energy Inelastic Neutron Scattering (HINS) at eV energies but now at low momentum transfers (q < 10 $Å^{-1}$). VLAD uses a novel neutron detection technique (n,γ-resonance detection) which was developed within the eVERDI Project (VESUVIO upgrade). Here, gamma detectors record the photon cascade following the resonant capture of the scattered neutrons by a thin ^{238}U foil. The γ-detector consists of a cerium doped Yttrium Aluminium Perovskite (YAP) scintillator coupled to a photomultiplier tube. With the current setup the accessibility of a yet

unexplored dynamical range of inelastic neutron spectroscopy at eV energies has been achieved, facilitating the investigation of electronic transitions in rare earth metals and compounds, vibrational levels in insulators, semiconductors, and magnetic materials.

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Title: Neutron Resonance Capture Analysis (NRCA) and Applications

Abstract:
Since the year 2000 neutron resonance capture has been applied as a method to analyse the bulk composition of objects using a time-of-flight (TOF) system at the GELINA facility in a joint project of the University of Delft and the EC-JRC IRMM in Geel (B). Neutron resonances occur at energies specific for isotopes and thus they are suitable to recognize elements of materials and objects. Short pulses (of ≈1ns) of 150 MV electrons from the electron linear accelerator of IRMM are stopped in a U-target to generate Bremsstrahlung, which in turn produces via photo-nuclear and fission reactions bursts of fast neutrons. The maximum repetition rate is 800 Hz. Subsequently these neutrons are slowed down (moderated) in water contained in two Be-tanks (4 cm thick) positioned close to the U-target. Several collimated beam tubes are viewing these tanks.
With flight paths of 13 and 29 m and the resolution available at the GELINA facility the practical range of neutron energies is from about 1 eV to about 5 keV for bronze objects. For determining the TOF the start pulse is extracted from the linac and the stop pulse is obtained from the detection of the prompt gamma radiation emitted after capture using a set of C_6D_6 detectors.
The elemental compositions of objects determined by NRCA have been used in a number of projects in collaboration with museums and university based archaeological institutes. For instance a series of bronze statuettes from a collection of Etruscan objects bought in 1826 and now owned by the National Museum of Antiquities in Leiden (NL) has been studied to verify their authenticity. On the basis of the zinc content it could be concluded that some of them were productions from a later period; probably from the Renaissance.
NRCA has also been used to study the composition of nuclear fuel material. It has been shown in a test NRCA experiment that the amount of gadolinium as a poison in uranium fuel material can be determined accurately.
NRCA is a fully non-destructive analytical method. The residual activation is negligible.

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