Microsymposia

MS.67.3

Quantum critical points and nematics: The ruthenate Sr$_3$Ru$_2$O$_7$

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Sr$_3$Ru$_2$O$_7$ is an interesting strongly correlated metal that can be tuned to show a zero temperature metamagnetic transition. In its vicinity, there is experimental evidence supporting the existence of a novel quantum phase, with anisotropic transport properties. In this talk, I will discuss this topics and describe an extensive follow-up project to characterise and understand this phase.

Keywords: magnetic phase transitions, magnetic properties, magnetic and transport behaviours

MS.67.4

Exotic superconductivity in crystals without inversion center

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I am planning to talk about some exotic properties in noncentrosymmetric superconductors which have no inversion symmetry in the crystal structure. The breakdown of inversion symmetry induces (i) the admixture of spin singlet and spin triplet order parameters, (ii) helical superconductivity, (iii) magneto-electric effect, and (iv) anomalous paramagnetic effect, and so on. Our microscopic theory on the noncentrosymmetric heavy fermion materials, namely CePt$_3$Si, CeRhSi$_3$ and CeIrSi$_3$ will be reviewed. The possibility of s+P-wave superconductivity is pointed out. I will discuss the relationship and common physics with FFLO superconductivity in heavy fermion superconductor CeCoIn$_5$, organic superconductors, cold fermion atoms and high density quark matters.

Keywords: superconductivity, noncentrosymmetry, magnetic properties

MS.67.5

Quantum mechanical delocalization of hydrogen atoms in (NH$_4$)$_2$PtCl$_6$

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We performed neutron diffraction on (NH$_4$)$_2$PtCl$_6$ using the JAEA single crystal diffractometer FONDER. The crystal was essentially in the ground state at 7 K. 59 (hkl) intensity data were MEM-analyzed. The resulting nuclear density is shown in the figure for the NH$_4^+$ portion of the structure. The four rings represent the protons forming an NH$_4^+$ ion. The hydrogen atom is delocalized on the ring of ca.0.08 nm in diameter. The orientation of the NH$_4^+$ ions is thus distributed over the ring in the ground state of the crystal. The distribution is evidence for rotational tunneling of NH$_4^+$ in the cubic environment, explaining the different low temperature behavior of (NH$_4$)$_2$PtCl$_6$ and (ND$_4$)$_2$PtCl$_6$.


Keywords: proton delocalization, ammonium ion, deuteration-induced phase transition

MS.68.1

On the evaluation of energy densities with aspherical pseudopotentials: A model study

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There is an increasing number of X-ray charge density studies reporting local and integrated kinetic-energy densities (KED) based on the pseudopotom model. These calculations utilize approximate KED functions and invoke the local virial theorem to derive the potential-energy density. Such a procedure thus combines a formalism of limited applicability with a density model lacking a physical soundness, through a relation that is known to be valid only for the exact properties in question. The purpose of this model study is to trace the propagation of errors associated with each step of the calculation. We evaluate a number of approximate KED’s using ab initio densities and their pseudopotom representations. The results are compared with the wave-function-based KED’s locally, as well as in terms of integrated values for atomic basins. We also test theoretical densities against the local virial relationship. In line with earlier observations, our analysis shows that KED’s obtained via functionals closely resemble exact KED’s only in regions of low and flat density. The discrepancy between exact and approximate KED

Keywords: quantum critical point, magnetic and transport behaviours.