European XFEL

THEORY GROUP MEETING

Thursday, 2 April 2015
11:00

AER 19 Seminar Room 4.14

Calculation of the X-ray absorption spectrum of $LaCoO_3$: exact diagonalization of cluster models

by

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I would like to present a brief introduction into the cluster-based approaches to calculation of various spectra of transition metal compounds. These spectra include X-ray absorption spectroscopy (XAS), resonant inelastic X-ray scattering (RIXS), photoemission spectroscopy (PES), inelastic neutron scattering, and others. Cluster models of the solid, comprised by a number of correlated d-shells, ligand shells, and core states, can be simplified by introduction of a special highly symmetric basis set (ligand orbitals). An efficient Lanczos exact diagonalization solver can be then applied to the resulting many-body Hamiltonian to reveal the ground state, as well as the response function for a given perturbation operator.

I also present some preliminary XAS spectra of $LaCoO_3$ calculated within the MeO_6-cluster approximation with hopping parameters derived from the first-principle electronic band structure (DFT).