Introduction to Spectroscopic Methods for Strongly Correlated Quantum Materials

May + June 2021
Physics Department / SBQMI - University of British Columbia

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The spectacular physical properties often observed in materials containing transition metal and rare earth elements challenge our comprehension of solid-state physics. These properties include unconventional superconductivity, unusually large magneto-resistance, metal-insulator transitions, heavy-fermion behavior, multiferroicity, "bad metal" behavior, amongst others. We would like to understand how the electrons in such materials interact with the lattice and *with each other* as to generate those intriguing quantum phenomena.

The standard approach in solid state physics is based on mean-field theories in which each electron moves in the periodic potential created by the average electron density resulting from the other electrons and the nuclei and is very successful for many solid-state materials. However, it fails badly for transition metal and rare earth based compounds. The reason is that the motion of *d*- and *f*-electrons are highly correlated, rendering us with a true hard-to-solve many-body problem. Nevertheless, in some cases one might hope to be able to describe the effect of these correlations in terms of an effective dressing of the electrons with a polarization cloud resulting in so called quasi particle behavior. The effective mass of the quasi particle reflects the influence of the dressing by the polarization cloud and can be very different from the bare or band mass.

This May + June 2021 lecture is part of a lecture series in which we will present a selection of spectroscopic methods that are very powerful for the determination of the electronic degrees of freedom of strongly correlated systems, with the objective to arrive at theoretical approaches or models that capture the essential mechanisms underlying the quantum properties of interest. We will look not only at the ground state but also (and in fact especially) at the excited states of the system. Here we would like to note that the ground state is perhaps a bit special since it basically has no properties except charge density and energy, while in contrast, most properties of a system involves an excitation of some form so that the study of excited states is a necessity for the understanding of the properties. We would like to add that a spectroscopy carried out at low temperatures involves a transition from the ground state and thus can infer information also about the ground state wave function.

The excited states can be charge neutral (inelastic neutron scattering, various forms of optical spectroscopy and electron energy loss spectroscopy, x-ray absorption and emission spectroscopy, (resonant) inelastic x-ray scattering), or with the system having electrons removed (photoelectron spectroscopy, scanning tunneling spectroscopy, Auger electron spectroscopy) or electrons added (inverse photoelectron spectroscopy, scanning tunneling spectroscopy). The excited states can span a wide range of energies, from meV to eV and even keV. The lower energy excitations may have the crystal momentum attached as a quantum number and are valuable in the search for the possible existence of quasi-particles. The higher energy excitations on the other hand, may be more atomic-like in nature and are powerful for

the identification of the bare particles and the dressing mechanisms that can explain the formation of quasi-particles.

We will start the May + June 2021 lecture with giving a few simple (but not too simple) illustrations that point the need to go beyond thinking in terms of one-electron states and energies when dealing with correlated systems. We need to work with many-electron states and total energies. This implies also that we no longer can use terms like (joint) density of one-electron states to describe spectroscopic data; instead we will use terms like spectral weights.

After this introduction, we will go in depth with the following spectroscopic methods: x-ray absorption spectroscopy, inelastic neutron scattering, inelastic x-ray scattering and Raman spectroscopy. We will explain the basic principles of these methods and we will describe the various experimental versions thereof. We will also give examples of their applications in modern day research on strongly correlated quantum materials. Recent advancements in the technical implementation of the methods are also part of this lecture.

In the subsequent lectures in 2022, we will discuss photoelectron and inverse electron spectroscopy, Auger electron spectroscopy, electron energy loss spectroscopy, and scanning tunneling spectroscopy.

Lecture schedule for May + June 2021:

Week 1 : May 10 - May 13 -- introduction: one-electron vs. many-electron states, H_2 molecule (ground state and excited states, exchange)
Week 2: May 17 - May 20 -- introduction: spectroscopy and spectral weights, H_2 molecule (photoemission, inverse photoemission)
Week 3: May 24 - May 27 -- x-ray absorption spectroscopy and dichroism, local atomic physics in solids, multiplets and crystal fields
Week 4: May 31 - June 3 -- core-level inelastic x-ray scattering: beyond dipole transitions, spectroscopy and imaging
Week 5: June 7 - June 10 -- inelastic neutron scattering
Week 6: June 14 - June 17 -- resonant inelastic scattering, Raman

Time schedule (tentative, to be discussed): 2 times a week, Tuesday + Thursday, 8:30-9:45 and 10-11:15 am UBC (5:30-6:45 and 7-8:15 pm Germany).

Office hours for informal questions and discussion can be arranged upon request.

ZOOM LINK:
https://zoom.us/j/7149396719
Meeting-ID: 714 939 6719
Passwort: 01187

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