Theory of Resonant Inelastic and Elastic X-ray Scattering by Magnetic Excitations and Ordering

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It has been long recognized that Resonant elastic X-ray Diffraction (RXD) at the Transition Metal $L_{2,3}$ edge is a very sensitive tool to measure magnetic ordering. The resonant enhancement of the scattering form factor is, by the optical theorem, related to the x-ray absorption spectral (XAS) function. Polarization and azimuthal dependence is given by the simple relation that the scattering cross section is proportional to: $F^{(0)}$ $(\varepsilon_{in} . \varepsilon_{out}^{*})$ + $F^{(1)}$ $(\varepsilon_{in} * \varepsilon_{out}^{*} .\mathbf{m})$ + $F^{(2)}$ $((\varepsilon_{out}^{*}.\mathbf{m})(\varepsilon_{in} .\mathbf{m})$-1/3$(\varepsilon_{in} .\varepsilon_{out}^{*}))$ [1]. This relation is however derived in spherical symmetry and strictly speaking only holds in spherical symmetry.
Within this talk I will show how these relations change when the real crystal symmetry is included and when these effects becomes important for real measurements [2].

Recently an amazing experimental progress has been made, which now makes it possible not only to measure elastic processes, but also Resonant Inelastic X-ray Scattering (RIXS) with such high resolution that single magnon excitations can be measured [3]. The theoretical understanding of these experiments is far from trivial. The resonant intermediate state contains a localized core hole which shows many-body interactions with the valence electrons. The magnon final state is dispersing and needs a description in momentum space. Purely local excitations can be understood [4] as well as collective excitations in d^9 systems [5], but generally collective excitations are problematic. One should realize that there is no theory that can include full many-body interactions on an infinite lattice. A sufficient understanding of RIXS might therefore seem hopeless
Within this talk I will present a solution to this problem. I present a tractable theory for the (RIXS) spectral function of magnons. The low-energy transition operator is written as a product of local spin operators times fundamental XAS spectra. This leads to simple selection rules for the magnetic cross section and to very similar relations as found for RXD [6].

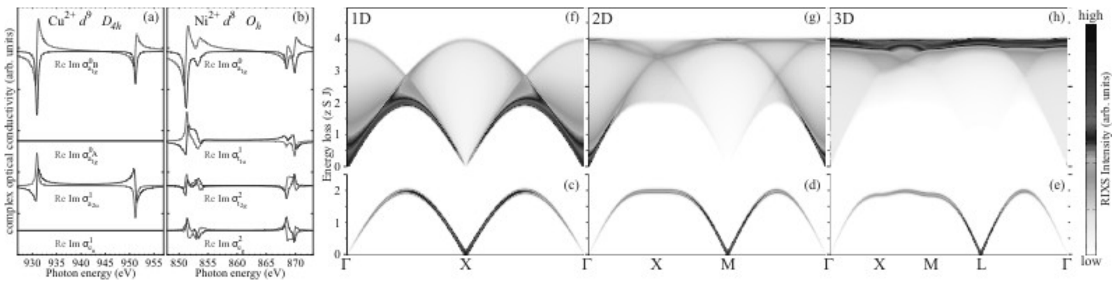

Fig 1) Left: Fundamental x-ray absorption spectra that enter in the RIXS transition operator as energy dependent complex matrix elements calculated for (a) Ni^{2+} and (b) Cu^{2+}. Right: The Cu^{2+} and Ni^{2+} one magnon (c,d,e) and Ni^{2+} two magnon (f,g,h) RIXS spectral function, calculated using linear spin-wave theory for a 1D chain (c,f), 2D square (d,g) and 3D cubic (e,h) Heisenberg model in energy loss units of $z\,S\,J$ (number of neighbors * spin * exchange constant).

References

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