**Supplementary information**

# Resonant inelastic X-ray scattering

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# RESONANT INELASTIC X-RAY SCATTERING

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## SUPPLEMENTARY INFORMATION

### INTERACTION OF X-RAYS WITH MATTER

The scattering of light from matter can be derived from Schrödinger's equation with the use of time dependent perturbation theory. The system without external light source defines the unperturbed state. The interaction between light and the electrons of a material is treated perturbatively. In linear order this yields the elastic scattering length as given by Kubo's formula. In second order this yields, with some slight modifications, the Kramers-Heisenberg equation describing the inelastic scattering of light.

Both in classical and in quantum physics, Maxwell's equations and the interaction between external electromagnetic fields and electrons are included into the Hamiltonian of a system by replacing the momentum of the electrons $\vec{p}$ with $\vec{p} - e\vec{A}$. In classical physics $\vec{A}$ is the vector potential defining the external magnetic and electric field. The constant $e$ is the charge of the electron. To quantize the electromagnetic field, the vector potential $\vec{A}$ can be expanded on a basis of plane waves inside a box with volume $V$. This yields a set of allowed modes with wave-vector $\vec{k}$ and polarization $\vec{\epsilon}$. We can write the vector potential $\vec{A}$ as an operator that can create or annihilate photons into the different plane wave modes:

$$\vec{A} = \sum_{\vec{k},\sigma} \sqrt{\frac{\hbar}{2\omega\epsilon_0 V}} \left( \vec{\epsilon_\sigma} b_{\sigma,\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \vec{\epsilon_\sigma^*} b_{\sigma,\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{r}} \right)$$

with the operators $b_{\sigma,\vec{k}}^\dagger$ and $b_{\sigma,\vec{k}}$ creating or annihilating a photon in the mode with wavevector $\vec{k}$, energy $\hbar\omega$ and polarization $\vec{\epsilon_\sigma}$. The quantum number $\sigma$ defines the two orthonormal vectors that form a basis for the polarization of the light. There are only two and not three polarization basis vectors as the polarization vector has to be perpendicular to the wavevector $\vec{k}$.

## COMPTON AND RAYLEIGH SCATTERING

In order to calculate the light scattered by a system we use time dependent perturbation theory. The Hamiltonian is split into two parts. The Hamilton operator $H_0$ contains all interactions of the system without external light field. The operator $H_1$ contains the change to the Hamiltonian due to the interaction with the external light field. To a good approximation (i.e. neglecting the interaction of the light with the atomic nuclei and neglecting the magnetic moment of the light) we find for the sum over all electrons:

$$H_1 = \sum_n \frac{1}{2m}\left(\vec{p_n} - e\vec{A}(\vec{r_n})\right)^2 - \frac{1}{2m}\vec{p_n^2}$$

$$= \sum_n \frac{e^2\vec{A}(\vec{r_n})^2}{2m} - \frac{e\vec{A}(\vec{r_n})\cdot\vec{p_n}}{m}$$

The operator $\vec{A}$ describes either the absorption or the emission of a photon. For scattering one needs a successive absorption and emission. In a time dependent perturbation expansion in operator $H_1$ scattering of light only happens if the operator $\vec{A}$ enters at least twice in the series expansion. This happens in first order perturbation theory for the operator $\overrightarrow{A^2}$ or in second order perturbation theory for the operator $\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}$. Scattering due to the $\overrightarrow{A^2}$ is known as Compton scattering Click or tap here to enter text. where the electric field is described as particles and one can have a picture of billiard balls scattering of each other taking into account energy and momentum conservation laws. Scattering due to the operator $\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}$ is related to Rayleigh scattering where the electromagnetic field induces an oscillating electric polarization of the system, which consequently leads to the emission of radiation.

## INELASTIC X-RAY SCATTERING

Inelastic light scattering due to the operator $\overrightarrow{A^2}$ is also known under the name of X-ray Raman Scattering (XRS) or non-resonant Inelastic X-ray Scattering (nIXS). Close to the atomic resonances in a material, i.e. at energies where a core electron can be excited to the unoccupied states just above the chemical potential, the resonant contribution dominates in intensity over the non-resonant contribution. Further away from the resonance the $\overrightarrow{A^2}$ scattering becomes the dominant channel for x-ray scattering. At small scattering angle, XRS can be described in the dipole approximation and its spectral shape is equivalent to X-ray absorption spectroscopy. At larger momentum transfer the dipole limit cannot be used and one can observe higher-order multipole transitions[275–278279]. This review deals with resonant IXS (RIXS). At resonance the scattering process is completely dominated by the operator $\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}$. and for the rest of this review we will neglect the $A^2$ interaction term.

66    The RIXS cross section is given by a second order response theory, which can be derived from second order
67    perturbation theory expanding the work of KuboClick or tap here to enter text. to second order. The double
68    differential cross section $\partial^2\sigma/\partial\Omega\partial\omega$ describes the scattering of a plane wave of light with wavevector $\vec{k_i}$ energy
69    $\hbar\omega$ and polarization $\vec{\epsilon_i}$.

70
$$\frac{\partial^2\sigma}{\partial\Omega\,\partial\omega} \propto -\mathrm{Im}\left(\left< i\left|R^{\overrightarrow{k_i},\overrightarrow{\epsilon_i}}_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}(\omega_i)^\dagger\, G(\omega)\, R^{\overrightarrow{k_i},\overrightarrow{\epsilon_i}}_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}(\omega_i)\right|i\right>\right)$$

71    The propagator $G(\omega)$ is defined as:

72
$$G(\omega) = \frac{1}{\hbar\omega + E_i + \mathrm{i}\frac{\Gamma}{2} - H} - \frac{1}{\hbar\omega - E_i + \mathrm{i}\frac{\Gamma}{2} + H}$$

73    The state |i> relates to the initial state or the ground-state of operator H with eigenenergy $E_i$. The operator $H$ is
74    the Hamiltonian of the full system without the applied electromagnetic field. It describes both the valence as
75    well as the core electrons. $\Gamma$ is the linewidth or self-energy operator of the excited state. The lifetime is state
76    dependent and as such $\Gamma$ is an operator. For practical calculations on finite Hilbert spaces $\Gamma$ has a finite value
77    due to Auger-Meitner and Fluorescence decay of the excited state.

78    The RIXS transition operator $R^{\overrightarrow{k_i},\overrightarrow{\epsilon_i}}_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}(\omega_i)$ describes the absorption of a photon with energy $\omega_i$, the propagation of
79    the photo-excited system and the subsequent emission of a photon with energy $\omega_o$. It is defined as a function of
80    the transition operators $T$ describe the absorption (emission) of a photon, and $\vec{r_n}$ is the position vector of electron
81    n:

82
$$R^{\overrightarrow{k_i},\overrightarrow{\epsilon_i}}_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}(\omega_i) = T^\dagger_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}\, G(\omega_i)\, T_{\overrightarrow{k_i},\overrightarrow{\epsilon_i}},\text{ with } T_{\vec{k},\vec{\epsilon}} \approx \frac{im\omega}{\hbar}\sum_n e^{i\vec{k}\cdot\vec{r_n}} b_{\vec{k},\vec{\epsilon}}\,\vec{\epsilon}\cdot\vec{r_n}$$

83    The propagator can be expanded on the eigen-basis of the Hamiltonian $H$

84
$$\sum_f\left|\left< f\left|T^\dagger_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}\frac{1}{\omega_i+E_i+i\Gamma/2-H}T_{\overrightarrow{k_i},\overrightarrow{\epsilon_i}}\right|i\right>\right|^2 = \sum_f\left|\sum_j\frac{<f|T^\dagger_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}|j><j|T_{\overrightarrow{k_i},\overrightarrow{\epsilon_i}}|i>}{\omega_i+E_i+i\Gamma_j/2-E_j}\right|^2.$$

85    By doing so one retrieves, in the limit where $\Gamma_f$ goes to zero, the Kramers Heisenberg equation

86
$$\frac{\partial^2\sigma}{\partial\Omega\,\partial\omega} \propto \sum_f\left|\sum_j\frac{\left< f\left|T^\dagger_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}\right|j\right>\left< j\left|T_{\overrightarrow{k_i},\overrightarrow{\epsilon_i}}\right|i\right>}{\omega_i + E_i + \mathrm{i}\frac{\Gamma_j}{2} - E_j}\right|^2 \delta(E_i + \omega_i - E_f - \omega_o)$$

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RIXS AS CONVOLUTION OF X-RAY ABSORPTION AND X-RAY EMISSION

92    RIXS can be viewed as the radiative x-ray emission intensities that are measured resonantly at an x-ray absorption
93    edge. If the interference effects are neglected, the intensity of the RIXS peak is the multiplication of the intensity
94    of the XAS excitation times the intensity of the XES decay.

95    $$\text{(eq. 4)} \sum_f \left| \sum_j \frac{<f|T^\dagger_{\vec{k}_o,\vec{\epsilon}_o}|j><j|T_{\vec{k}_i,\vec{\epsilon}_i}|i>}{\omega_i + E_i + i\Gamma/2 - E_j} \right|^2 = \sum_f \sum_j <f|T^\dagger_{\vec{k}_o,\vec{\epsilon}_o}|j>^2 <j|T_{\vec{k}_i,\vec{\epsilon}_i}|i>^2$$

96    In some cases, one may also neglect the core hole effect and describe the RIXS process using only one-electron
97    transitions. The equation can then be further simplified to [53]:

98    $$\frac{\partial^2 \sigma}{\partial \omega_o \, \partial \omega_l} \propto \int_\varepsilon d\varepsilon \, \frac{\rho(\varepsilon)\rho'(\varepsilon + \hbar\omega_{in} - \hbar\omega_{out})}{(\varepsilon - \hbar\omega_{out})^2 + \frac{\Gamma_n^2}{4}}$$

99    with $\rho$ and $\rho'$ the occupied and unoccupied density of states. This equation makes the RIXS process very
100   accessible to theoretical modelling. However, the challenge is to assess when the approximations can be applied.

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103   MOMENTUM DEPENDENCE IN RIXS

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105   In order to discuss the momentum dependence in RIXS it is useful to factorize the momentum dependence into
106   a structure factor and atomic scattering lengthClick or tap here to enter text.. The structure factor depends on
107   the positions of the atoms, the atomic scattering length depends on the type of atom and its environment. For a
108   molecule or solid with atoms at position $\vec{R_j}$ we can define the RIXS operator as:

109   $$R^{\vec{\epsilon}_i,\vec{\epsilon}_o}_{\vec{q},\omega_i} = \sum_J e^{i\vec{q}\cdot\vec{R_J}} R^{\vec{\epsilon}_i,\vec{\epsilon}_o}_{J,\omega_i}$$

110   The RIXS operator $R^{\vec{\epsilon}_i,\vec{\epsilon}_o}_{\vec{q},\omega_i}$ makes coherent excitations with energy $\hbar\omega = \hbar(\omega_i - \omega_o)$ and momentum $\hbar\vec{q} =$
111   $\hbar(\vec{k_i} - \vec{k_o})$. These are a result of excitations made at and around site $J$ by the operator $R$ coherently summed
112   over all lattice sites $J$ at position $\vec{R_j}$ with the phase factor $e^{i\vec{q}\cdot\vec{R_J}}$. Note that this operator depends on $\vec{k_i}$ and $\vec{k_o}$. If
113   the wavelength $2\pi/|\vec{k}|$ is large compared to the radial extend of the local core state excited, one can use the
114   dipole approximation and set $e^{i\vec{k}\cdot\vec{r}} \approx 1$, removing the momentum dependence from the local RIXS transition
115   operator. This is for most edges a good approximation. Note that for deep core levels the incident energy is high,
116   and thus the wavelength short. At the same time the radial extend of the core orbital is small such that the dipole
117   approximation is still good.

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121    RIXS is, for many cases, comparable to Inelastic Neutron Scattering (INS). Both methods allow one to probe the
122    energy and momentum dependence of low lying excitations. These include phonons, magnons and crystal-field
123    transitions i.e. orbitons. The RIXS cross section is often larger, allowing one to probe much smaller sample
124    volumes. On the other hand, the maximum momentum transfer in RIXS is set by the resonant photon energy.
125    Often this only includes part of the Brillouin zone. As such both methods are complementary. There is one big
126    difference between RIXS and INS. For INS the interaction with the neutron and the (magnetic moment) of the
127    electrons is well understood and relatively simple. In RIXS the low energy excitations are made in a resonant
128    process by the operator $R_{J,\omega_i}^{\overrightarrow{\epsilon_i},\overrightarrow{\epsilon_o}}$. This operator includes the interaction with the electromagnetic field (light) twice.
129    The interaction between electrons and photons is just like the interaction between neutrons and electrons well
130    understood. The operator $R_{J,\omega_i}^{\overrightarrow{\epsilon_i},\overrightarrow{\epsilon_o}}$ also includes the propagator $G(\omega)$. This propagator describes the (Fourier
131    transform) of the time evolution of the many-electron system after a photon is absorbed. This propagator
132    includes a local core hole and all many-body interactions between the electrons. As core states are localized one
133    can calculate this propagator relatively well. However one does need advanced multi-refference quantum
134    chemistry methods to do this. As a result nothing is simple about this propagator.

135    The operator $R_{J,\omega_i}^{\overrightarrow{\epsilon_i},\overrightarrow{\epsilon_o}}$ can excite single, double, triple, etc. spin flips at and around site $J$, it can make charge
136    excitations and measure the charge dynamical structure factor, it can excite phonons. Actually any low energy
137    excitation that is allowed by symmetry can be excited by RIXS. The intensity of the different excitations RIXS
138    couples to is strongly polarization $(\overrightarrow{\epsilon_i}, \overrightarrow{\epsilon_o})$ and resonant energy $\omega_i$ dependent. For many choices of polarization
139    and resonant energy, only a few low energy excitation types dominate the RIXS spectrum.

140    In order to understand which low energy excitaiton the RIXS operator $R_{J,\omega_i}^{\overrightarrow{\epsilon_i},\overrightarrow{\epsilon_o}}$ can excite one can expand the
141    operator on a complete orthonormal set of simpler operators. The expansion coefficients then will carry the
142    resonant energy and polarization dependence. For a doped Hubbard model, relevant for the cuprates this yields
143    a set of spin and charge operators acting at and around site $J$, with specific energy and polarization dependence[50].
144    For magentic excitations one can expand the RIXS operator onto spin operators. In spherical symmetry expanded
145    to local spin excitations on site J only this yields[21].

$$146 \qquad R_{J,\omega_i}^{\overrightarrow{\epsilon_i},\overrightarrow{\epsilon_o}} = \sigma^{(0)}(\omega_i)\overrightarrow{\epsilon_i} \cdot \overrightarrow{\epsilon_o}^* + \frac{1}{s}\sigma^{(1)}(\omega_i)\overrightarrow{\epsilon_o}^* \times \overrightarrow{\epsilon_i} \cdot \overrightarrow{S_J}$$

$$147 \qquad + \frac{1}{s(2s-1)} \sigma^{(2)}(\omega_i)\left( (\overrightarrow{\epsilon_i} \cdot \overrightarrow{S_J})(\overrightarrow{\epsilon_o}^* \cdot \overrightarrow{S_J}) + (\overrightarrow{\epsilon_o}^* \cdot \overrightarrow{S_J})(\overrightarrow{\epsilon_i} \cdot \overrightarrow{S_J}) - \frac{2}{3}(\overrightarrow{\epsilon_i} \cdot \overrightarrow{\epsilon_o}^*)\overrightarrow{S_J}^2 \right),$$

148    With s the length of the local spin operator and $\sigma^{(0)}(\omega_i)$ the local isotropic x-ray absorbtion spectrum, $\sigma^{(1)}(\omega_i)$
149    the local magnetic circular dichroic x-ray absorbtion spectrum one would measure if the spin was fully aligned
150    and, $\sigma^{(2)}(\omega_i)$ the local magnetic linear dichroic x-ray absorbtion spectrum one would measure if the spin was
151    fully aligned. For atoms at lower crystal point-group symmetries the operators branch according to the point-
152    group branching rulesClick or tap here to enter text.. The expansion of the RIXS operators into polynomials of the
153    spin operators (Stevens Operators) truncates in spherical symmetry at order 2. For lower symmetries, which
154    crystals always posess, the series does not truncate as angular momentum can be transferred to the crystal

155    lattice[21]. For resonant energies below the main absorbtion line the local transitions normally dominate the
156    spectrum. For resonant energies that are at or above the first resonance, one can expect that additional spin
157    excitations on the neighboring sites around lattice site J become important.

## DIRECT AND INDIRECT RIXS

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160    In the results section we classified different RIXS spectra into core and valence RIXS. This classification depends
161    on the question if the final state of the RIXS process has a core hole or not. For valence RIXS one needs to consider
162    polarization, resonant energy, and momentum transfer to fully understand the spectra. For core RIXS one can
163    neglect the momentum transfer as core levels do not disperse. A different classification of the RIXS process can
164    be made based on the interactions involved within the RIXS process. One can classify both core and valence RIXS
165    into direct or indirect RIXS.

166    For direct RIXS a core electron can be excited into one of the single electron states above the chemical potential.
167    After the excitation another electron can decay from one of the occupied single electron states, either a shallow
168    core electron or a valence electron, into the previously formed core hole. For indirect RIXS one also starts by
169    exciting a core electron into one of the single electron states above the chemical potential. One now assumes
170    that the electron that decays back into the core is the same electron as the electron that was excited. This
171    seemingly elastic process can generate excitations. The core hole and additional electron interact with the other
172    electrons in the system. This can result in the scattering of other electrons from occupied to unoccupied orbitals,
173    thereby generating low lying excitations.

174    One has to be careful when explaining direct and indirect RIXS in terms of decaying with the same or a different
175    electron. Electrons are indistinguishable particles and formally one cannot distinguish if the same or a different
176    electron decayed compared to the one excited. A more accurate definition of direct and indirect RIXS can be
177    made by the use of a Dyson perturbation expansion

178    We can write the full Hamiltonian $H$ of the system as a sum of $H_0$ and $H_1$

179    $$H = H_0 + H_1,$$

180    with $H_0$ the (mean-field) Hamiltonian describing the ground-state without core hole and $H_1$ all terms neglected
181    in $H_0$ to obtain the full Hamiltonian. For the case where $H_0$ is a full interacting Hamiltonian describing the valence
182    electrons including the many-body Coulomb corrections the Hamiltonian $H_1$ contains the direct and exchange
183    interaction between the valence electrons and the core hole. For the case where $H_0$ is a mean-field Hamiltonian,
184    as assumed in many discussions on direct and indirect RIXS, the operator $H_1$ also contains the two electron
185    Coulomb interactions between the valence electrons. Once an appropriate choice for $H_0$ and $H_1$ is made we can
186    rewrite the RIXS operator $R_{\vec{k}_o,\vec{\epsilon}_o}^{\vec{k}_i,\vec{\epsilon}_i}(\omega_i)$ in terms of a direct and indirect part. The RIXS operator $R_{\vec{k}_o,\vec{\epsilon}_o}^{\vec{k}_i,\vec{\epsilon}_i}(\omega_i)$ is given
187    by the product of an operator that absorbs an x-ray and creates a core hole ($T_{\vec{k}_i,\vec{\epsilon}_i}$), an operator that describes
188    the propagation of the many electron core hole state in the system ($G(\omega_i)$), and an operator that emits an x-ray
189    and fills the core hole ($T_{\vec{k}_o,\vec{\epsilon}_o}^{\dagger}$),

190
$$R^{\overrightarrow{k_\iota},\overrightarrow{\epsilon_\iota}}_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}(\omega_i) = T^\dagger_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}\, G(\omega_i)\, T_{\overrightarrow{k_\iota},\overrightarrow{\epsilon_\iota}}.$$

191 Using the definition of the Green's function we find for the Dyson equation

192
$$
\begin{aligned}
G^{-1}(\omega_i) \; &= \hbar\omega + E_i + i\frac{\Gamma}{2} - H \\
&= \hbar\omega + E_i + i\frac{\Gamma}{2} - H_0 - H_1 \\
&= G_0^{-1}(\omega_i) - H_1,
\end{aligned}
$$

193 and thus, by multiplying from the left with $G_0(\omega_i)$ and from the right with $G(\omega_i)$

194
$$G(\omega_i) = G_0(\omega_i) + G_0(\omega_i)H_1\, G(\omega_i).$$

195 We now can write for the direct RIXS operator

196
$$Rd^{\overrightarrow{k_\iota},\overrightarrow{\epsilon_\iota}}_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}(\omega_i) = T^\dagger_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}\, G_0(\omega_i)\, T_{\overrightarrow{k_\iota},\overrightarrow{\epsilon_\iota}},$$

197 and for the indirect RIXS operator

198
$$Ri^{\overrightarrow{k_\iota},\overrightarrow{\epsilon_\iota}}_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}(\omega_i) = T^\dagger_{\overrightarrow{k_o},\overrightarrow{\epsilon_o}}\, G_0(\omega_i)H_1\, G(\omega_i)\, T_{\overrightarrow{k_\iota},\overrightarrow{\epsilon_\iota}}.$$

199 The distinction between direct and indirect RIXS can be exemplified by two cases.

200 For direct RIXS an effective operator can be derived that only depends on the polarization of the light. If one
201 assumes that $H_0$ only includes the core level onsite energy and spin-orbit coupling interaction one obtains the
202 fast collision approximation. This name originates from the observation that if the interaction of the photon with
203 the system occurs very fast, no additional indirect excitations are made. The fast collision approximation is a
204 reasonable approximation if the intermediate state Coulomb interaction and crystal field is small compared to
205 core hole lifetime. One can use this approximation for excitations within the $t_{2g}$ orbitals excited at the $L_{23}$ edge
206 in Iridates for example. In this limit one can derive an analytical expression for the RIXS scattering cross section
207 and its polarization dependence, thereby relating RIXS to inelastic neutron scattering. The effective operator
208 formalism described in the previous section includes these direct RIXS processes, but also includes the indirect
209 RIXS processes and as such has a dependence of the RIXS cross section on the resonant light energy.

210 Indirect RIXS becomes important, for example, at transition metal K edges. At these edges one can excite a core
211 s electron into the p sub-shell of a transition metal ion. Subsequently this p electron decays back to the core
212 orbital. In the intermediate state the p electron can interact with the d electrons via the Coulomb interaction.
213 One could for example excite with $x$ polarized light an $s$ core electron to the $p_x$ orbital. Coulomb interaction then
214 can scatter the $p_x$ electron to a $p_y$ electron whilst simultaneously scatter a $d_{yz}$ electron to an $d_{xz}$ orbital. The $p_y$
215 electron can subsequently decay back to the s core state under the emission of a photon with $y$ polarization.

216 In general the RIXS intensity is given by a sum of the direct and indirect part as well as interferences between the
217 two channels. One should be carefull when making a series expansion of $H$ in $H_1$ around $H_0$. There is no

218     guarantee that such a series converges. We note that in this definition of direct and indirect RIXS, each RIXS
219     feature in the multiplet model (for example $3d^7 > 2p^53d^8 > 3d^7$) will be a combination of direct RIXS and indirect
220     RIXS. If one does not use a single-electron model for $H_0$, but instead uses that $H_0$ is the crystal field multiplet
221     model then all multiplet states will be direct RIXS and charge transfer states could be called indirect RIXS. But if
222     the Anderson impurity model is defined as $H_0$ then everything becomes again direct RIXS. In other words, the
223     distinction between direct and indirect RIXS depends on the model that is chosen for $H_0$ and $H_1$.

224
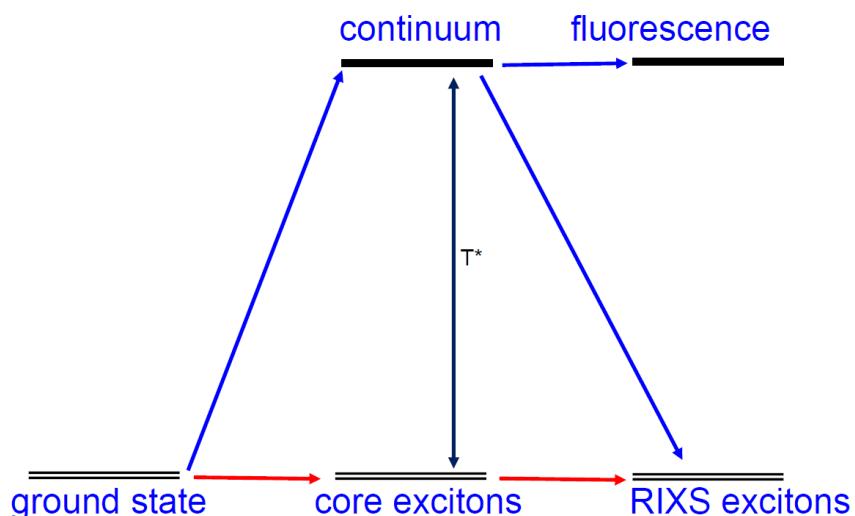


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226     **Figure S1: Direct and indirect RIXS channels due to interference of excitons and continuum excitations.**

227     For gas phase molecules one can make a distinction between excitons ($H_0$) and ionization ($H_1$) and for the K edge
228     of transition metal systems one can make a distinction between core excitons ($H_0$) and continuum excitations
229     ($H_1$). Figure S1 gives an example of direct and indirect RIXS for such system. The RIXS experiment that follows the
230     path from the ground state to core excitons and then decay to RIXS excitons would be direct RIXS. Indirect RIXS
231     would be a continuum excitation followed by decay to the RIXS excitons. The reason that indirect RIXS is possible
232     is due to the coupling of the core excitons ($H_0$) and the continuum ($H_1$).

233