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# MULTIELECTRON TRANSITIONS ON X-RAY ABSORPTION SPECTROSCOPY

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During the photoabsorption process in a N electrons atom, the hole potential V acts as a time-dependent perturbation on the remaining N-1 "passive" electrons. Due to this perturbation each of these electrons, initially in a state $|i\rangle$, can make a transition to a state $|f\rangle$ with a probability $w_{fi}$ given by:

$$w_{fi} = 1/\hbar^2\omega_{fi}^2 \left| \int \partial V_{fi}/\partial t \exp(i\omega_{fi}t)\, dt \right|^2 \qquad (1)$$

where $\omega_{fi}=(E_f-E_i)/\hbar$ and $V_{fi}=\langle f|V|i\rangle$.

If the change of the potential during the core hole excitation is slow compared to $\omega_{fi}^{-1}$ (adiabatic limit) the integral in eq.(1) becomes small and the transition probability negligible.

Since in the X-ray absorption spectroscopy the adiabatic limit is usually reached, the single particle picture is considered enough to describe the photoabsorption process.

However there is evidence that in many systems there are significant many-body effects which must be taken into account for a full explanation of the absorption edge structures (XANES and EXAFS). These effects can be viewed as "noise", obscuring the study of important one electron features and also as a tool to discover and understand many-body interactions.

We have investigated many-body effects in the absorption spectra of rare gases (Ar, Kr and Xe) and of some liquid and solid Rb compounds, and we have found spectral features which can be explained as two electron transitions to discrete or continuum states.

In particular, for the first time the structures above the Kr K edge have been interpreted as due to multielectron transitions involving K,

M and N electrons[1]. The cross section of one of these transitions has been analysed and a "turn-on" more rapid than the one expected according to a time dependent treatment[2] has been found. The observed behaviour agrees quite well with the prediction of a model proposed by Stohr, Jaeger and Rehr[3], based on the exchange interaction. This model, however, is based on several approximations and can't be considered of general validity.

Our results, together with the ones on Ne[4] and Ar[5], show that many-body effects play an important role also in the adiabatic limit, and that in this limit electrons interaction, which must be better understood, can enhance the multielectron transition cross sections respect to the independent particle model previsions.

The role of the passive electrons on the EXAFS region was emphasized by Stern et al.[6] to explain the reduction of the experimental EXAFS amplitude respect to the theoretical one, obtained through single particle calculations. However up to now the possibility that passive electrons can add structures to the EXAFS ones has not been explicitly considered.

Our experimental results on liquid and solid Rb compounds show that strong structures due to multielectron transitions are present in the EXAFS region. These structures introduce anomalous frequencies on EXAFS which give rise to "non structural" peaks in the Fourier transform.

To remove the possible "noise" in the structural inversion procedure and to understand completely the many-body processes in the adiabatic limit, more data on multielectron transition cross sections of various systems should be obtained and more accurate models developed. Furthermore, to perform a correct data analysis the most suitable procedure for the subtraction of the atomic background must be selected.

References:

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