J. At. Mol. Sci.
doi: 10.4208/jams.040715.050915a

Vol. **6**, No. 2, pp. 137-144
June 2015

# A graphic method for computing multi-atomic resonant photoemission cross section

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Received 7 April 2015; Accepted (in revised version) 9 May 2015
Published Online 6 June 2015

**Abstract.** A graphic method for studying multi-atom resonant photoemission process in molecules and solids is presented in this work. The Feynman diagrams have been applied to describe the interactions between atoms in MnO molecules. The theoretical results show that the resonant contribution exhibits a strong distance-independent and element specific effects for the neighboring atoms. Two mechanisms, the interactions between the atoms and the reabsorption process have been supposed in the present work to explain the multi-atomic resonant photoemission for the first time.

**PACS**: 32.80.Fb, 32.80.-t, 3380E

**Key words**: multi-atomic resonant photoemission; electronic correlation effect; Feynman diagram.

## 1 Introduction

The cross section of the multi-atomic resonant photoemission receives contributions from two main channels, the direct photoionization and the resonant photoionization channels [1]. The characteristics of the two parts are obvious due to different interaction operators, different symmetry selection, polarization and angular distribution properties [1-3]. The intensity of the direct photoionization channel is related to a transition element which, in the dipole and one-particle approximation, is given by a dipole transition element between the ionized core orbital and a continuum orbital [2]. The resonant part depends instead on a resonance-continuum hamiltonian matrix element which, in the independent particle approximation, may be reduced to a two-electron integral involving the core orbital, the continuum orbital, the bound virtual orbital of the core excitation and the bound ionized orbital [1]. Recently, the multi-atomic resonant photoemission has

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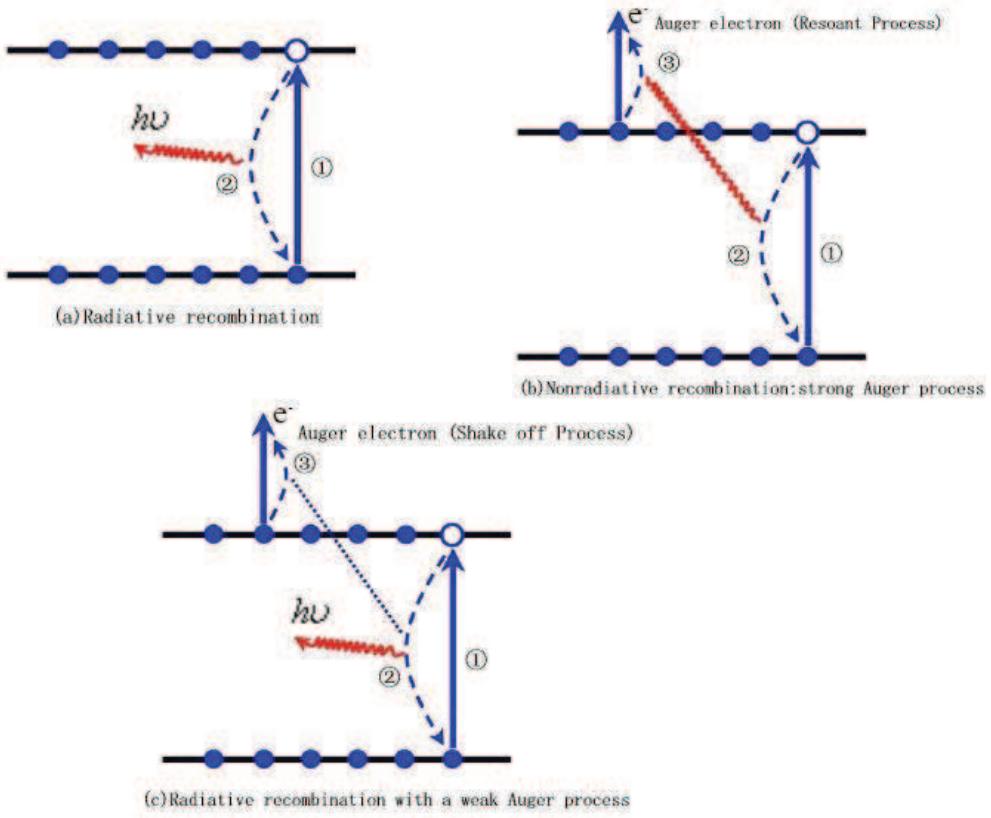


Figure 1: The photoemission processes of the multi-electron excitation for single atom resonance.

been found in MnO solid without the theoretical confirmation. It is the main object of the present study to estimate quantitatively the resonant intensity with the Feynman diagram of two electron matrix element which contains two core orbitals strongly localized at different atomic sites. The diagram rules describing the electron interaction in one atom have been extended into the interaction between the electrons of the nearby atoms.

The well-known intra-atomic single-atom resonant photoemission (SARPE) [2] has been generalized to apply to multi-atomic resonant photoemission (MARPE) [1] in the present work. In the photoabsorption of atoms, the existence of the multi-electron excitation process has been known for a long time. The mechanism of multi-electron excitation in photoabsorption can be considered due to shake-up and shake-off processes as shown in Fig. 1. When an inner-shell vacancy is created by photoabsorption, another atomic electron is excited to an unoccupied bound state in the shake-up process, while it is ejected into the continuum in the shake-off process. Such ionization and excitation processes in inner shell electrons far above threshold have been extensively studied [1-11].