Mechanisms of giant resonance in 4d photoionization of Eu

X. M. Tong, D. Kato, T. Watanabe, and S. Ohtani

Cold Trapped Ions Project, ICORP, JST, Axis 3F, 1-40-2 Fuda Chofu, Tokyo 182-0024, Japan
Tel: +81-0424-83-1094, Fax: +81-0424-83-1409, E-mail: tong@hci.jst.go.jp

Giant resonance in rare-gas photoionization process has been a subject of interest for a long time [1, 2]. The broad resonance of 4d electron photoionization cross section for rare gas atoms can be explained as being due to the electron-electron dynamic correlation and the double-well potential for the final f partial wave [2]. There are also many experimental studies [1, 3] of the 4d photoionization cross sections for rare-earth atoms. The shape of giant resonance for rare earth atoms is different from that of the rare gas atoms due to the occupation of 4f electrons. The giant resonance shape of Eu atom is a typical example of the rare-earth atoms since the 4f orbit is half-filled. Experiments [3] show that the width of giant resonance for Eu atoms is narrower than that of the rare gas atoms and the line profile of the resonance is strongly asymmetry, similar to the Fano-profile [4] of autoionization state. Although the time-dependent local density approximation (TDLDA) has been successfully used to explain the giant resonance for rare gas atom [5], which is a spin-paired system, it is difficult to study Eu atom by TDLDA since Eu atom is a highly spin polarized system. The 4d photoionization cross section of Eu atoms has been studied by many body perturbation theory (MBPT). The MBPT calculations showed that the $4d^9 4f^8$ level is above the $4d^9 4f^7$ threshold. This causes a giant resonance in the 4d photoionization cross-section [6]. Such MBPT calculated photoionization cross-section is much narrower than the experimental observation [3].

To investigate the detail mechanisms of the giant resonance in 4d photoionization process of Eu, we have performed a theoretical investigation of the photoionization process for Eu 4d electrons by time-dependent local spin density approximation method (TDLSDA) with the optimized effective potential and self-interaction correction [7, 8]. In the calculations, we have decomposed the contribution of spin-up and spin-down electrons. Fig. 1 shows the decomposed results for spin-up and spin down electrons. It is interesting to see that there is a relative broad resonance for spin-down electron and a very sharp resonance for the spin-up electron (the f-electrons are in the spin-up state). The peak positions of the two resonance are separated by 5 eV. When we switch on the interaction between the spin-up and spin-down electrons, due to such quasi-bound state interaction with a continuum state, the giant resonance is formed with a line shape of Fano-profile. Note, the original Fano-profile is due to a bound state (with zero width) interaction with a continuum state. The line width of autoionization states is of the order of meV. Here, the giant resonance of Eu 4d electrons is due to a quasi-bound state (with width of eV) interaction with a continuum state. The line width of giant resonance is about 10 eV, much larger than that of the autoionization states. Our calculated results of the 4d photoionization cross section are in good agreement with experiments [3] (filled circles in Fig. 1). Since it is a relative measurements, we scaled the experimental data to our data. To compare with the experimental data, the photon energy is shifted by a 4 eV. [This shift is

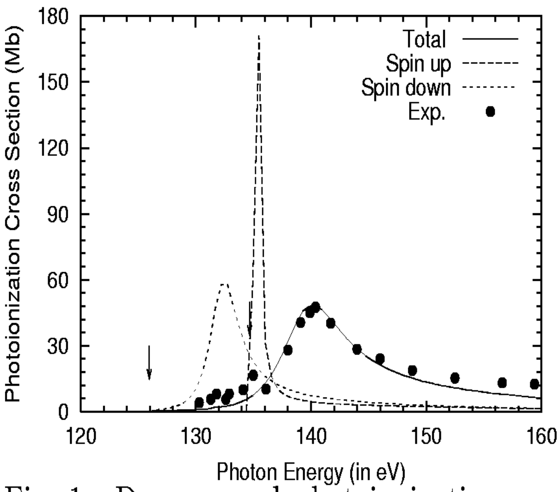

Fig. 1. Decomposed photoionization cross sections of 4d electrons from Eu atoms.

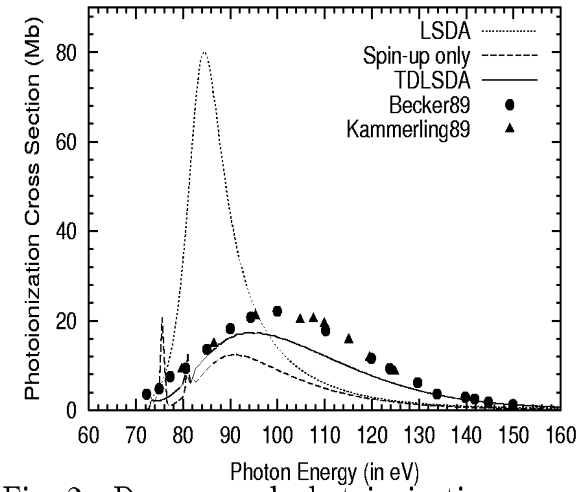

Fig. 2. Decomposed photoionization cross sections of 4d electrons from Xe atoms.

originated from difference of the calculated 4d binding energy with the exact binding energy.].

We have also performed a same calculation for rare gas Xe atom as shown in Fig. 2. Different from Eu case, a giant resonance appears even in the LSDA calculation although the calculated shape is quite different from the experiments [9, 10]. The TDLSDA results show a great improvement. [Note, the photon energy is shifted by 7 eV.] Since the spin-up and spin-down 4d electrons move in the same effective potential, we only plot the spin-up contribution in Fig. 2. The peak of the photoionization is shifted by the interaction of spin-up and spin-down electrons. We do not observe a clearly Fano profile in the photoionization cross section due to the spin-up and spin-down channels are identical. Such results support above discussion for giant resonance in Eu atoms.

To summary, we have studied the photoionization process of 4d electrons for Eu by linear density response method. By decomposing the contribution of the 4d electron in spin-up and spin-down states, we clearly identified the line profile in the giant resonance is due to the broad resonance of 4d spin-down electrons interacting with a sharp resonance of 4d spin-up electrons.

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