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Effect of Interchannel Coupling and Confinement on the Photoionization of Kr

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Synopsis: The effect of interchannel coupling and confinement on the photoionization of the Kr atom is examined. It is found that the position of the Cooper minimum is sensitive to interchannel coupling in both free and confined Kr. The strengths of the confinement oscillations are also sensitive to interchannel coupling.

A confined quantum system such as an atom trapped in a fullerene cage has been an area of much interest in recent years [1-3]. It has stimulated a wide range of studies in physics, chemistry and also in interdisciplinary areas such as material science, nanoscience etc. [4].

In this work we study the effect of interchannel coupling on the photoionization of the 4p, 4s, 3d and 3p subshells using the relativistic random phase approximation (RRPA) [5].

The fullerene potential which encapsulates the atom is simulated by a spherical annular shell potential:

$$V(r) = \begin{cases} -U_0 & for \quad r_c \leq r \leq r_c + \Delta \\ 0 & otherwise \end{cases}$$

where r_c=5.8 a.u. is the inner radius, Δ=1.9 a.u. is the thickness of the shell and $U_0 = 0.302$ a.u. is the depth of the potential [2].

The effect of interchannel coupling is studied by carrying out the RRPA calculations at different levels of truncation for both free Kr and confined Kr (@Kr). A comparison of the results at different levels of truncation demonstrates the effects of coupling additional channels at each level.

As an example, the 4s photoionization cross-section of both free Kr and @Kr at the three levels of truncations; (i) two channels arising from 4s (ii) seven channels from 4p and 4s (iii) 18 channels from 4p, 4s, 3d and 3p are shown in Fig.1. The Cooper minimum (CM) is below the 4s threshold in the two channel calculations. Interchannel coupling moves the CM to above the threshold of 4s for both free Kr and @Kr.

The position of the CM is unaffected by the confinement at all levels of truncation, indicating that confinement is not involved in the dynamics causing the CM. In addition, it is seen that the amplitudes of the confinement oscillations are affected by interchannel coupling.
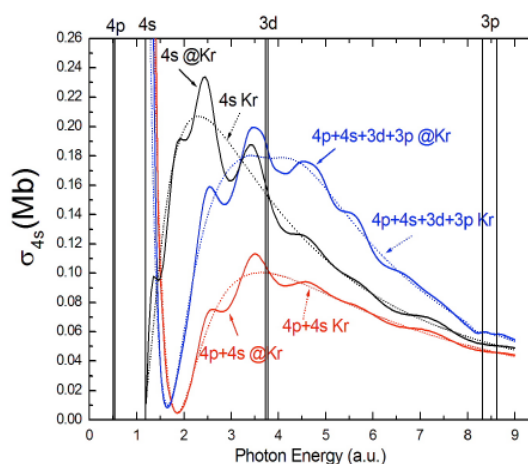

Figure 1. 4s photoionization cross-sections for free and @Kr for three levels of truncation of RRPA: (i) 2 channel intra-shell 4s coupling, (ii) 7 channels from 4p+4s and (iii) 18 channels from 4p+4s+3d+3p. Vertical lines show the ionization threshold energies for the various subshells of Kr.

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