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Theoretical characterization of the collective resonance states underlying the xenon giant dipole resonance

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Synopsis We present an *ab initio* theoretical characterization of the two fundamental collective resonances underlying the xenon giant dipole resonance (GDR). This is achieved consistently by two complementary methods implemented within the many-body configuration-interaction singles (CIS) theory. We identify one resonance at an excitation energy of 74 eV with a lifetime of 27 as, and the second at 107 eV with a lifetime of 11 as. Insights on the nature of these resonances are provided, as well as information on previously unknown resonances in xenon.

The xenon GDR is not only a well-studied spectroscopic feature but also the key to understanding many start-of-the-art experiments on xenon exposed to strong midinfrared lasers or free-electron lasers. While the photoabsorption spectrum associated with the GDR has been characterized remarkably well, a question frequently overlooked is what exactly are the fundamental modes giving rise to the GDR.

We present a complete theoretical characterization of the resonance substructures underlying the xenon GDR. This is achieved consistently by two complementary methods implemented using CIS. The first method directly diagonalizes the many-electron Hamiltonian using the smooth exterior complex scaling technique. The second one involves a new application of the Gabor analysis to wave-packet dynamics.

We identify one resonance at an excitation energy of 74 eV with a lifetime of 27 as, and the second at 107 eV with a lifetime of 11 as. These excitation energies are expected to be more accurate than those given in the pioneering work of Wendin [1], since no approximate condition is invoked here to find the resonances. We demonstrate that many-body correlations result in qualitatively different substructures of the GDR: upon including the interchannel couplings between the $4d$ electrons, there are two far-separated resonances instead of three close-lying modes (see Fig. 1). As the wave functions of the two resonances are not dominated by any single particle-hole state, they correspond to plasma-like collective oscillations of the $4d$ shell as a whole.

Although the two resonances cannot be disentangled in the one-photon absorption cross section, a recent experiment at the free-electron laser FLASH, using an XUV nonlinear spectroscopy technique, has provided the first direct evidence for the two collective dipolar resonances [3]. Thus, it may be expected that experiments of this kind will offer an opportunity to test the results presented here.

In addition to the two resonances described above, we predict a new type of giant resonances in xenon. These new resonances have a total angular momentum larger than one, so they can only be accessed through multiphoton processes. This opens up possibilities to probe new quantum structures of matter with modern light sources.

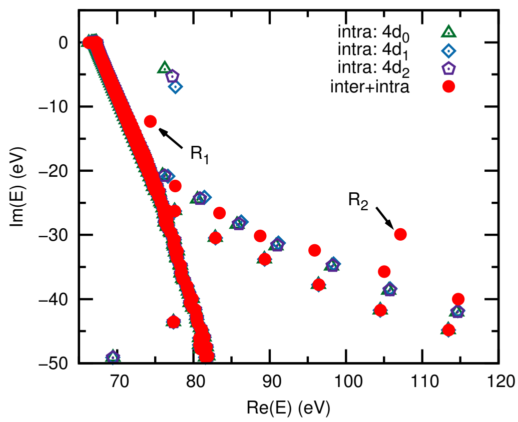

Figure 1. Complex energy spectra of the many-body Hamiltonian for the intrachannel ("intra") and full CIS ("inter+intra") models. From Ref. [2].

References

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