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On the computations of decay widths of Fano resonances[1]
TSVETA MITEVA, SÉVAN KAZANDJIAN, NICOLAS SISOURAT, Université Pierre et Marie Curie, Paris — We present a novel approach to the calculation of decay widths of Fano resonances in singly-ionized systems. In our approach, the bound part of the resonance is approximated at the zeroth order as a one-hole configuration. The final states of the decay are obtained after diagonalization of the Hamiltonian matrix in the space of all two-hole-one-particle (2h1p) configurations with a fixed virtual orbital. The Fano-CI method can be applied to the computation of both total and partial decay widths. Furthermore, it has fairly low computational costs and can thus be employed for investigating medium-sized atomic and molecular systems. To check the validity of our method, we carried out benchmark calculations of Auger and ICD widths of small rare-gas and hydrogen-bonded clusters. Comparison with available theoretical and experimental data shows that a satisfactory estimate of the decay width can be achieved with a relatively small basis set, which is of importance for the application of the method to larger systems. [1] [1] T. Miteva, S. Kazandjian and N. Sisourat, accepted in Chem. Phys. (2016)

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