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2009 J. Phys.: Conf. Ser. 194 152013

(http://iopscience.iop.org/1742-6596/194/15/152013)

Journal of Physics: Conference Series **194** (2009) 152013 doi:10.1088/1742-6596/194/15/152013

Complete Feshbach-type projection method to compute autoionizing states in Li-like atomic systems

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Synopsis A fully *ab initio* method of solution to compute autoionizing states in Li-like atomic systems based on the application of the Feshbach projection formalism is proposed. Applications of the Feshbach formalism, which in principle is a complete many-particle theory, to systems of more than two-active electrons are very scarce due to the limitations imposed by the practical construction of correct projection operators $\mathcal{P}$ and $\mathcal{Q}$ inherent to the theory. We include rigorously all the ingredients required by the Feshbach theory in order to compute accurate resonance parameters for the lowest autoionizing states of Li and Ne^{7+}, for the $^2S^e$, $^2P^o$ and $^2D^e$ symmetries.

Auger decay from metastable states with core holes is receiving a new deal of attention in view of new experiments that reveal the excitation and relaxation dynamics of core-excited atoms [1] or the localization of inner holes in molecules [2] by using ultrafast probing with attosecond pulses. These experimental advances call for theoretical methods to efficiently compute and describe autoionizing states in many-electron atoms and molecules in both stationary and dynamical pictures.

In this communication we revisit the Feshbach formalism and apply it to compute autoionizing states in three-electron atoms. For closed channel resonances the Feshbach projection-operator formalism [3] provides a rigorous procedure for decomposing the total wave function Ψ into its (square-integrable) resonant $\mathcal{Q}$ and (scattering-like) nonresonant $\mathcal{P}$ parts in order to compute resonant parameters. The explicit construction of complete Feshbach projection operators $\mathcal{P}$ and $\mathcal{Q}$ for systems containing more than two electrons has posed practical difficulties. Thus, previous applications have made use of quasi-projectors for which the condition of idempotency inherent to any projection operator is relaxed (see Ref. [4] and references therein). Since previous applications of quasi-projectors have led to resonance parameters in reasonable agreement with experiments, further elaborations were not pursued. In this work we explicitly include all the required ingredients of the Feshbach theory. First, we introduce the full $\mathcal{P}$ projector, as described by Feshbach, by solving algebraically a related integral equation. This guarantees idempotency for the operators and the correct asymptotic behaviour for $\mathcal{Q}\Psi$ and $\mathcal{P}\Psi$. The $\mathcal{Q}$-projected Schrödinger equation is solved with a Phillips-Kleinman pseudopotential approach, which is formally equivalent, to avoid the explicit construction of the $\mathcal{Q}$ projector. Also, the generalized optical potential is included to solve the $\mathcal{P}$-projected Schrödinger equation.

The target eigenfunction to be included in the $\mathcal{P}$ projector is computed in terms of 40 configurations built with optimized STOs functions. Eigensolutions of the $\mathcal{QHQ}$ problem are computed in terms of $\sim$ 10000 three-electron configurations built with uncorrelated STOs basis, which are then used also to expand the optical potential. The nonresonant $\mathcal{P}\Psi$ functions are constructed through an static exchange scheme using the same target eigenfunction. Energy positions, Auger widths and energy shifts are then computed. To illustrate the performance of our approach we provide resonance parameters for the lowest autoionizing states in two different cases within the Li-like series, Li and Ne^{7+}, for the $^2S^e$, $^2P^o$ and $^2D^e$ symmetries.

References

[1] Drescher M *et al.* 2002 *Nature* (London) **419** 803; Kienberger R *et al.* 2004 *Nature* (London) **427** 817; Wickenhauser M *et al.* 2005 *Phys. Rev. Lett.* **94** 023002

[2] Schöffler M S *et al.* 2008 *Science* **320** 920

[3] Feshbach H 1962 *Ann. Phys.* **19** 287

[4] Temkin A and Bathia A K, in *Autoionization: Recent Developments and Applications*, edited by Temkin A (Plenum Press, New York, 1985), pp. 1-72

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