# Solving time-(in)dependent Schrödinger equation with Smolyak scheme using a system-bath like partition

David Lauvergnat*[1]

[1]Institut de Chimie Physique, Bâtiment 349, Université Paris-Saclay, 91405 Orsay Cedex France – CNRS : UMR8000, Université Paris-Saclay,Sorbonne Universités – France

**Abstract**

Solving the Schrödinger equation using method using a multidimensional grid such as DVR, FBR-DFR or pseudo-spectral approaches (1) is limited by the number of degrees of freedom, $d$, of the system. With these methods using direct-product, the numerical complexity grows exponentially with $d$ and it is relatively easily to study four (d=6) or five (d=9) atomic systems. This limit can be pushed away using contraction techniques (2-4), pruned basis sets (5) or schemes with a basis function selection. (6)
Somehow, the Smolyak scheme (7-9) can be viewed as an approach with a selection of basis functions and a sparse grid adapted to that basis set. The parameter, $L$, controls the selection and thus the size of the basis set and the grid. With this scheme, the numerical complexity grows as a polynomial of degree $L$ with $d$. Therefore, systems up to 12 degrees of freedom can be studied, (10-12) although larger systems (d=21) are possible if few states are needed.(13)

This limit can be pushed away using a system-bath separation, and in our Smolyak scheme, three $L$parameters are required: (14) (i) $Ls$ for the degrees of freedom associated with the system part. (ii) $Lb$ associated with the bath mode. (iii) Lm a parameter controlling the coupling between the system and the bath.

This system-bath separation has no limitation with respect to the form of the Hamiltonian and it works well when the coupling between the system and the bath is weak and typically: Ls $>>$ Lb and Lm $>$ Ls (Lm=Ls+1 or Ls+2 can be used).

To illustrate the advantages and the limitations of this approach, time-independent and time-dependent applications are presented:

- The effect of the rotation-translation motions (bath modes, up to 120) of the water shell on the rotation-translation H2 motions (system modes, 5) in clathrate hydrate. (14)

- The photoisomerization of a retinal chromophore model with 2 active modes (system) and 23 modes (bath). (15)

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*Speaker

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