The Abdus Salam
International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

Workshop on
NEW TRENDS IN QUANTUM DYNAMICS AND ENTANGLEMENT
21 - 25 February 2011

Hierarchical Effective-mode Decomposition for non-Markovian Quantum Environments

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Abstract:

This talk summarizes our recent developments of reduced-dimensional representations of non-Markovian environments, based upon the construction of a set of effective environmental modes [1-4]. These effective modes, which are generated by suitable coordinate transformations from spin-boson type models, absorb the cumulative effects of the system-bath coupling and can be shown to reproduce the short-time dynamics exactly. Furthermore, inclusion of residual modes bilinearly coupled in a Mori chain type description successively accounts for the dynamics on longer time scales [2]. Termination of the chain by coupling the final chain member to a Markovian bath yields a representation of non-Markovian system-bath dynamics that converges to the exact dynamics as the chain is extended to higher orders. We have further shown that truncation of the chain at successive orders generates a family of approximate spectral densities which approach the true spectral density with increasing accuracy [2,4]. Convergence can be explicitly demonstrated in terms of the properties of the residual spectral densities which approach a quasi-Ohmic limit [4]. Overall, the approach thus provides a very general strategy for the embedding of non-Markovian environments into an enlarged set of variables. An extension to correlated environmental fluctuations is straightforward. Applications are presented for non-adiabatic dynamics and excitation energy transfer in extended molecular systems [1,3]. Here, decoherence is typically found to set in with a delay, beyond the shortest time scale which is determined by few effective modes.