Hierarchical equations of motion for quantum dissipation and quantum transport

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In the mesoscopic world the nano-structured environment is not just of quantum in nature but also often nonperturbative and non-Markovian for its influence on the system of primary interest. In this talk, I will discuss the hierarchical equations of motion (HEOM) approach [1–4] that can be considered as a fundamental formalism in quantum mechanics of dissipative and open systems.

HEOM is formally equivalent to such as the Feynman-Vernon influence functional and nonequilibrium many-body Green's function formalisms [5], but numerically more implementable. It provides a unified treatment of various decoherence and quantum transport processes. It renders also a unified view on various existing approximated theories, such as the quantum master equation and stochastic Liouville equation [6], and consequently, often further results in some simple but important modifications to those conventional approximations [7].

I will also discuss about two recent developments, the best/minimum stochastic environment basis set for optimal HEOM construction [8] and the efficient on-the-fly numerical filtering algorithm [9], that significantly enhance the numerical tractability of the exact HEOM dynamics. Numerical results on the 2D spectrum of a model light harvesting antenna system and the quantum transport through Anderson model quantum dots system will be presented.

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