A Time-dependent Multi-reference Unified Cluster Cumulant Formulation to Study the Subdynamics of Quantum System Coupled both to Thermal and Stochastic Bath

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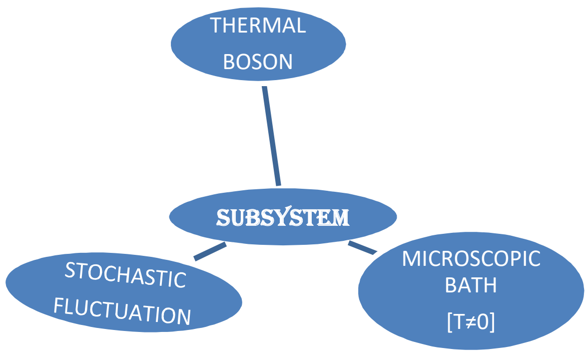

Abstract

This is to introduce a time-local effective hamiltonian unified cluster cumulant method based on the Time-dependent Multi-reference Cluster Cumulant (TDMRCC) and Thermal Cluster Cumulant (TCC) strategy developed by Mukherjee and his coworkers [13-17]. A factorized ansatz for $U_I P = [U_I]_{ex}[U_I]_M P$ with $P = |\varphi_i> \otimes |0_\beta> \otimes |0_f>$, where $|\varphi_i>$, $|0_\beta>$ and $|0_f>$ denote the purely quantum mechanical vacuum state, the thermal vacuum state, the base state for the solvent degrees of freedom respectively, and $[U_I]_{ex}$ consists of operators admixing the thermally as well as the stochastically projected **model space** functions with that of the **virtual space** outside the model space whose functions govern the time-evolution of $[U_I]_M$ via the time-local effective operator, $V_{eff}[\beta, \xi, t]\ (=<< V_I[U_I]_{ex} >_\beta>_f)$, where $< \cdots >_\beta$ and $< \cdots >_f$ denote thermal and stochastic averaging respectively. The exponential ansatz is introduced both for $[U_I]_{ex}$ and $[U_I]_M$ and these ansatze are normal ordered with respect to both the thermal and the stochastic variables, i.e., $[U_I]_{ex} = \left\{\left\{e^{S^f_{m,n}}\right\}_\beta\right\}_f$ and $[U_I]_M = \{e^{X_{k,k}}\}_\beta$. The averaged evolution operator, $<< U_I(t) >_\beta>_f$ with respect to both the thermal boson variables in thermal equilibrium and the stochastic variables is obtained. Finally, the mathematical expression for the second order cluster cumulant $[X_{0,0}]^{(2)}$ is derived for a quantum particle trapped in a 1-dimensional anharmonic oscillator potential coupled both to the stochastic and thermal baths.