Path integral Liouville dynamics for real time dynamics & a unified framework for path integral molecular dynamics for quantum statistics

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We first show a unified second-order scheme for constructing simple, robust and accurate algorithms for typical thermostats for exact quantum/classical statistics for the canonical ensemble. The scheme consistently improves the efficiency for evaluating all quantum thermodynamic properties for any type of thermostat. Even when the Born-Oppenheimer approximation is broken, the unified scheme offers a powerful and accurate tool for studying non-adiabatic systems in thermal equilibrium.
In the second part of the talk, we show a new imaginary time path integral based method—path integral Liouville dynamics (PILD) in the Wigner phase space. PILD offers a potentially useful approach for molecular systems to have the two important properties: conserves the quantum canonical distribution and recovers exact thermal correlation functions (of even nonlinear operators, i.e., nonlinear functions of position or momentum operators) in the classical, high temperature, and harmonic limits. Some applications to water, ammonia, methane, zundel cation, and liquid para-hydrogen will be demonstrated.

References

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