Direct calculation of thermal and time-dependent properties from a normal-ordered exponential ansatz. A unified perspective: Electronic, Vibrational, Vibronic, Magnetic

Marcel Nooijen

University of Waterloo

The direct calculation of thermal properties (e.g. partition function) and time-correlation functions for systems that have many contributing states is an interesting topic that has received considerable attention recently. I will discuss a normal ordered exponential ansatz to parameterize thermal (or time-dependent) density matrices and/or time-correlation functions where appropriate. When applied to fermions, e.g. the electronic structure problem, the theory at zero temperature reduces to the cumulant version of the contracted Schrödinger equation. When applied to vibrational problems the theory is exact for single state quadratic (or harmonic) potentials, but it is also applicable to non-adiabatic vibronic models, providing access to spectra through the time-correlation function. We will also discuss a version that is applicable to magnetic model hamiltonians, focusing on thermal properties. The emphasis of this presentation is on the unversality of the approach, and applications to a range of fairly simple model systems.