Numerical Evidence Invalidating Finite-Temperature Many-Body Perturbation Theory

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Several low-order perturbation corrections to the grand potential and internal energy of a molecule at a finite temperature are determined numerically as the \( \lambda \)-derivatives of the respective quantity calculated exactly (by thermal full configuration interaction) with a perturbation-scaled Hamiltonian, \( H_0 + \lambda V \) (\( \lambda \) is a coupling constant) as

\[
X^{(n)} = \frac{1}{n!} \frac{\partial^n X}{\partial \lambda^n} \bigg|_{\lambda=0}.
\]  

The data thus obtained serves as a benchmark against which analytical formulas can be validated. The first- and second-order corrections from finite-temperature many-body perturbation theory based on Matsubara Green’s function [1] disagree with these benchmark data, calling into question the validity of this theory discussed in a number of textbooks [2, 3, 4]. The renormalized finite-temperature perturbation theory by Hirata and He [5] is also found to be incorrect.

References