Vibrational auto-adjusting perturbation theory

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In this work a new method to calculate anharmonic vibrational ground and excited state energies is proposed. The method relies on the auto-adjusting perturbation theory (APT) which has been successfully used to diagonalize square matrices. We use as zero-order correction the self-consistent vibrational energies, and with the APT approach we calculate the vibrational anharmonic correlation correction to any desired order. In this talk we present the methodology and apply it to a model system and formaldehyde. Vibrational APT approach shows a robust convergent behavior even for the states where the standard (Rayleigh–Schrödinger) vibrational Møller–Plesset perturbation theory is clearly divergent.