

Accurate computations of vibrational energies and vibrational spectra of molecules require an inclusion of the anharmonic forces. In standard computational protocols, a large vibrational Hamiltonian matrix is diagonalized, and spectral intensities are calculated for individual transitions separately. In this work we propose an alternate direct generation of the spectral curves based on a temporal propagation of a trial vibrational wavefunction followed by a Fourier transformation. The lack of the lengthy and computer-memory demanding diagonalization makes the method suitable for larger molecules. It is especially convenient for sparse Hamiltonians that are commonly obtained within the harmonic oscillator basis set, and the algorithm is amendable to parallelization. On a model water dimer basic convergence properties are discussed. The method is then applied to vibrational Raman intensities of the fenchone compound, where it provides spectral shapes comparable with those obtained by the classical approaches.