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Computing alignment and orientation of non-linear molecules at room temperatures using random phase wave functions SHIMSHON KALLUSH, Department of Physics and Optical Engineering, ORT Braude College, SHARLY FLEISCHER, School of Chemistry, Tel Aviv University, ULTRAFAST TERAHERTZ MOLECULAR DYNAMICS COLLABORATION — Quantum simulation of large open systems is a hard task that demands huge computation and memory costs. The rotational dynamics of non-linear molecules at high-temperature under external fields is such an example. At room temperature, the initial density matrix populates $\sim 10^4$ rotational states, and the whole coupled Hilbert space can reach $\sim 10^6$ states. Simulation by neither the direct density matrix nor the full basis set of populated wavefunctions is impossible. We employ the random phase wave function method to represent the initial state and compute several time dependent and independent observables such as the orientation and the alignment of the molecules. The error of the method was found to scale as $N^{-1/2}$, where N is the number of wave function realizations employed. Scaling vs. the temperature was computed for weak and strong fields. As expected, the convergence of the method increase rapidly with the temperature and the field intensity.

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