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Efficient time evolution of thermal ensembles by Hilbert space sampling

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Coherent control of bond making in chemical reactions has recently been successfully demonstrated under thermal conditions. In this experiment, pairs of magnesium atoms were made to collide at a temperature of around 1000 K and were subsequently excited into electronically excited states by a femtosecond laser pulse. The resulting UV emission signal proved to be a clear indicator of the formation of magnesium dimers. The current theoretical framework to describe this experiment models the thermal ensemble of magnesium atoms via random phase wavefunctions. Although this proves to yield significantly reduced numerical effort compared to a full description of the thermal density matrix, time propagation still proves to be the crucial computational bottleneck. We aim to alleviate this bottleneck by investigating the possibility to sample the Hilbert space not randomly but systematically via eigenstates of the Hamiltonian. It turns out that using this eigenstate-based sampling minimizes the worst-case error among arbitrary observables if no a priori information on the dynamics is available. We systematically benchmark the computational effort to obtain accurate estimations on observables both via random-phase sampling and via eigenstate-based sampling.

Primary author: HEGER, Marec (Universität Kassel)

Presenter: HEGER, Marec (Universität Kassel)

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