Quantum Scrambling in Molecules

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In quantum systems, out of time order correlators (OTOCs) can be used to probe the sensitivity of the dynamics to perturbing the Hamiltonian or changing the initial conditions ordinarily associated with classical chaos or its quantum analog. The vibrations of polyatomic molecules are known to undergo a transition from regular dynamics at low energy to facile energy flow at sufficiently high energy. Molecules therefore represent ideal quantum systems to study the transition to chaos in many-body systems of moderate size (here 6 to 36 degrees of freedom). By computing quantum OTOCs and their classical counterparts we quantify how information becomes 'scrambled' quantum mechanically in molecular systems. We show cases where molecules exhibit good quantum-classical correspondence of OTOC and cases where this correspondence fails to hold due to quantum localization. We also compare quantum scrambling rate in our system with Maldacena bound. Our results suggest even at chemical energy and with dozens of vibrational degree of freedom, many molecules scramble information about their initial state slowly, which opens up room for optical control of chemical reaction when OTOC remains sufficiently small.