VISTA Seminar

Seminar 11

9:30 – 11:00 am EST / 2:30 – 4:00 pm GMT / 3:30 pm – 5:00 pm Paris

TOC:

On the dynamical origins of nonstatisticality

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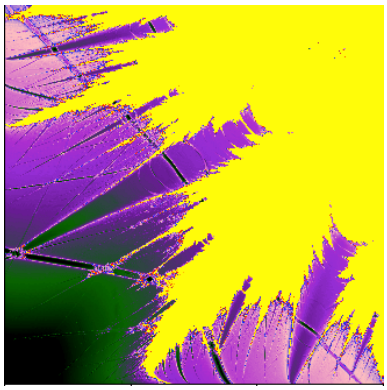

In systems undergoing non statistical reaction dynamics, the phenomenon of intramolecular vibrational energy redistribution (IVR) takes on a centre stage. In fact, obtaining the correct reaction mechanism and performing mode-specific chemistry require the identification of the preferred energy flow pathways. In order to identify the dominant IVR pathways one needs to identify the various anharmonic resonances and map out their connectivity at the energy of interest. Fundamentally, it is transport over this network of resonances, also known in the nonlinear dynamics setting as the Arnold web, that is ultimately required to understand the transition to statisticality as well. For isolated molecules with three or more degrees of freedom this presents a formidable challenge.

In this talk I will present our results [1] on the onset of statisticality in unimolecular reactions using the models proposed [2] by Don Bunker nearly half a century ago. Our study builds on the early work of Oxtoby and Rice [3] and brings out the key features on the resonance network that regulate the energy flow dynamics. A feature of particular interest is the so called resonance junction wherein several independent resonances intersect. Such junctions, somewhat counterintuitively, act as local dynamical traps that result in high correlated dynamics and the possible decoupling of a subset of the vibrational modes over chemically significant timescales. This talk provides evidence for the role of such junctions in the observed non-statistical dynamics. I will, time permitting, briefly discuss the significance [4,5] of the dynamical traps to the quantum ergodicity transition [6] and the scaling picture [7] of quantum IVR dynamics.

References

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Simulation of quantum molecular dynamics with analog quantum computers

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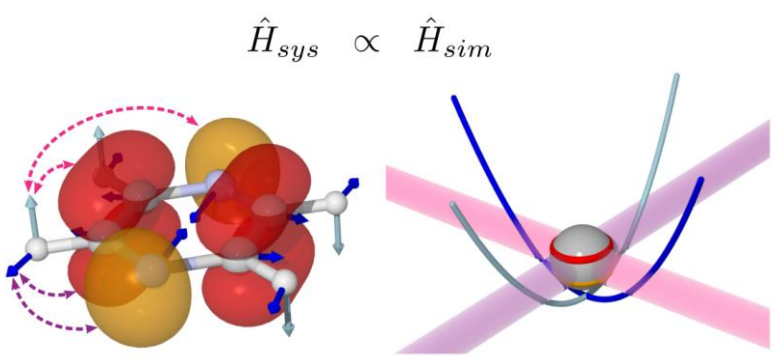

Quantum simulation is a challenging task for modern computers due to the exponential growth of information, often requiring approximations to the wavefunction and its evolution to adequately reduce the computational cost. Universal quantum computers may be used to simulate quantum systems with a significantly lower scaling, but current technologies have proven incapable of exceeding the success of quantum chemical approaches on classical computers in the near future [1–3]. An alternative approach to quantum simulation is the use of analog quantum computers, whereby the Hamiltonian of a desired molecule or material is mapped onto a controllable quantum system [4,5]. We focus on the simulation of ultrafast photochemistry and excited-state dynamics with vibronic coupling model Hamiltonians. Our approach [6] leverages the bosonic degrees of freedom present in certain quantum computing architectures, such as trapped ions. Using two laser interactions with a single trapped ion, we are capable of simulating a two-state, two-mode linear vibronic coupling model, such as that of pyrazine. The simulation can be extended to open quantum systems with tunable system-bath coupling using one additional laser field. Our approach readily scales to greater numbers of electronic and nuclear degrees of freedom, with the potential for full quantum mechanical simulation exceeding the ability of classical computers using current technology.

References:

[1] A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, and M. Head-Gordon, *Science* **2005**, *309*, 1704–1707.
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