Analog quantum simulation of quantum chemical dynamics with a trapped-ion system

Ting Rei Tan
C. H. Valahu, V. C. Olaya-Agudelo, R. J. MacDonell, T. Navickas, A. D. Rao, M. J. Millican, Tim F. Wohlers-Reichel, J. B. Pérez-Sánchez, J. Yuen-Zhou, M. J. Biercuk, I. Kassal.

The University of Sydney, Sydney, Australia
tingrei.tan@sydney.edu.au

Abstract

Quantum computers (QC) promise to solve computational challenges in chemistry by requiring only linear resource scaling. However, almost all chemical applications of QC have focused on *static* molecular properties, usually energies, making them unsuitable for addressing chemical *dynamic* problems, especially in strong vibronic (vibrational + electronic) coupling regimes where the Born-Oppenheimer approximation breaks down. Here, we show that vibronic Hamiltonians representing ultrafast molecular dynamics can be scalably and efficiently simulated on a mixed qudit-boson (MQB) simulator that provides order-of-magnitude resource savings compared to conventional qubit-only approaches [1]. We performed two experiments in a programmable trapped-ion MQB simulator. First, shown in Fig. 2, we observed geometric-phase interference in the dynamics of a nuclear wavepacket travelling around an engineered conical intersection [2]. Second, we extended the MQB approach to predict the molecular vibronic absorption spectrum of a sulphur dioxide molecule, see Fig. 2 [3]; our method offers better scalability by performing quantum simulation in the time domain; the number of required measurements depends on the desired spectral range and resolution, not molecular size.

References

[1] R. J. MacDonell *et al.*, Chem. Sci., **12** (2021) 9794.
[2] R. J. MacDonell *et al.*, Chem. Sci., **14** (2023) 9439.
[3] C. H, Valahu *et al.*, Nat. Chem., **15** (2023) 1503.
[4] D. M. P. Holland *et al.*, Chem. Phys. **118** (1994), 317.

Figures

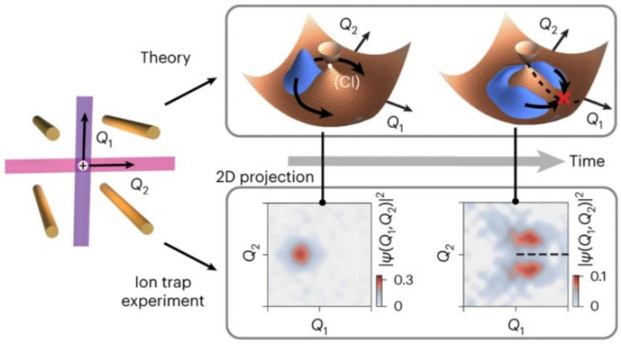

Figure 1: We performed a trapped-ion experiment directly detecting a geometric phase in dynamics around a conical intersection (CI). Our results track the wavepacket evolution dynamics, revealing the clear destructive interference as the wavepacket originally displaced from the CI (at $t = 0$) encircles the CI at $t = T$. Our work demonstrated remarkable hardware efficiency; we performed using a single trapped ion to solve a problem that otherwise would have required many qubits on a qubit-based QC.

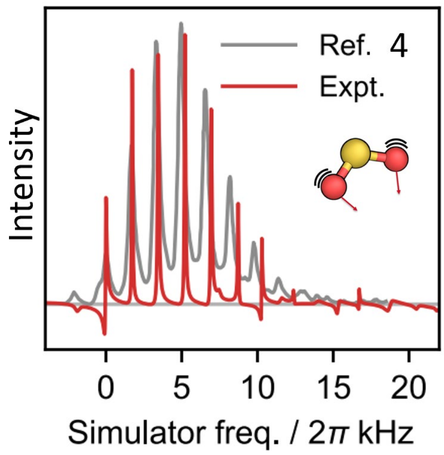

Figure 2: We predict the vibrational-electronic spectrum of a sulphur dioxide (SO2) molecule (red) with exceptional accuracy when compared to the spectroscopically observed spectrum at 320 K (grey).