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Analogue quantum simulation of molecular vibronic spectra with a trapped ion

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The analogue simulation of a quantum chemical system is challenging using conventional computers, particularly in strong vibronic (vibrational and electronic) coupling regimes when the Born-Oppenheimer approximation breaks down. The vibronic terms in Hamiltonians representing ultrafast molecular dynamics can be efficiently simulated on quantum systems with coupled internal states and bosonic modes [1]. We can use this mapping to recast basic molecular dynamics onto our 171Yb+ ion system. The radial motional modes of the ion behave as the vibrational modes of the molecule, while the necessary molecular interactions are implemented using a pair of Raman beams carrying multiple frequency tones.

We implemented the analogue quantum simulation in a proof-of-principle experiment to reconstruct molecular spectra. We found the quality of the simulations were limited by the dephasing of the motional modes. The source of dephasing was found to be the voltage noise of the radio-frequency trapping field. By implementing amplitude noise filtering and feedback, we improved radial mode coherence times from ˜1 ms to more than ˜30 ms. This enabled us to compute the 1-dimensional Franck-Condon spectra of an SO2 molecule [2] and demonstrate geometric phase effects in molecular dynamics [3].

[1] Analog quantum simulation of chemical dynamics. Ryan J. MacDonell, Claire E. Dickerson, Clare J. T. Birch, Alok Kumar, Claire L. Edmunds, Michael J. Biercuk, Cornelius Hempel and Ivan Kassal, Chem. Sci., 2021,12, 9794-9805
[2] Predicting molecular vibronic spectra using time-domain analog quantum simulation. Ryan J. MacDonell, Tomas Navickas, Tim F. Wohlers-Reichel, Christophe H. Valahu, Arjun D. Rao, Maverick J. Millican, Michael A. Currington, Michael J. Biercuk, Ting Rei Tan, Cornelius Hempel, Ivan Kassal, arXiv:2209.06558
[3] Direct observation of geometric phase in dynamics around a conical intersection. Christophe H. Valahu, Vanessa C. Olaya-Agudelo, Ryan J. MacDonell, Tomas Navickas, Arjun D. Rao, Maverick J. Millican, Juan B. Pérez-Sánchez, Joel Yuen-Zhou, Michael J. Biercuk, Cornelius Hempel, Ting Rei Tan, Ivan Kassal, arXiv:2211.07320

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