Analog Quantum Simulation of Non-Condon Effects in Molecular Spectroscopy

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In my talk, I will present a linear optical implementation for analog quantum simulation of molecular vibronic spectra [1], incorporating the non-Condon scattering operation with a quadratically small truncation error. To date, analog and digital quantum algorithms for achieving quantum speedup have been suggested only in the Condon regime, which refers to a transition dipole moment that is independent of nuclear coordinates. For analog quantum optical simulation beyond the Condon regime (*i.e.*, non-Condon transitions), the resulting nonunitary scattering operations must be handled appropriately in a linear optical network. In our recent paper [2], we consider the first- and second-order Herzberg–Teller expansions of the transition dipole moment operator for the non-Condon effect for implementation on linear optical quantum hardware. We believe that the method opens a new way to approximate arbitrary nonunitary operations in analog and digital quantum simulations. We report silico simulations of the vibronic spectra for naphthalene, phenanthrene, and benzene to support our findings.

References

[1] J Huh, G G Guerreschi, B Peropadre, J R McClean and A Aspuru-Guzik, Nat. Photon. **9**, 615 (2015)

[2] H Jnane, N P D Sawaya, B Peropadre, A Aspuru-Guzik, R Garcia-Patron and J Huh, ACS Photonics, DOI:10.1021/acsphotonics.1c00059; arXiv:2011.05553 (2021)