ESI Erwin Schrödinger International Institute for Mathematics and Physics

universität wien

DVR 0065528

Seminar

Dr. Wojciech Roga

National Institute of Information and Communications Technology,

Tokyo

Molecular vibronic spectra from boson sampling and compressive sensing

Friday, October 18, 2019

at 11:00 h

ESI, Boltzmann Lecture Hall

Abstract: Probabilities of vibronic transitions in molecules are referred to as Franck-Condon factors (FCFs). Although several approaches for calculating FCFs have been developed, such calculations are still challenging. Recently it was shown that there exists a correspondence between the problem of calculating FCFs and boson sampling [1]. However, if the output photon number distribution of boson sampling is sparse then it can be classically simulated [2]. Exploiting these results, we develop a method to classically approximately reconstruct the distribution of FCFs of certain molecules. We first obtain the marginal photon number distributions for pairs of modes of a Gaussian state associated with the molecular transition. We then apply a compressive sensing method so-called polynomial-time matching pursuit to recover FCFs [3]. We discuss when this method stops to be efficient classically. Moreover, an idea how to apply quantum computing to general compressive sensing problems is shortly discussed.

[1] J. Huh, G. G. Guerreschi, B. Peropadre, J. R. McClean, and A. Aspuru -Guzik, Boson sampling for molecular vibronic spectra, Nature Photonics 9 615 (2015).
[2] W. Roga, M. Takeoka, Classical simulation of boson sampling with sparse output, arXiv:1904.05494 (2019).
[3] K. Valson Jacob, E. Kaur, W. Roga, M. Takeoka, Franck-Condon factors via compressive sensing, arXiv:1904.05494 (2019).

R. Zeier

October 11, 2019