Seminar

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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.

R. Zeier

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