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An application for Gaussian Boson Sampling: vibronic spectra of molecules

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Abstract

In recent years, quantum informatics has gained considerable recognition in the world of scientific research. At the same time, the concept of the qubit also became common knowledge, which is nothing more than an abstraction of an arbitrary two-state quantum system. It is characterized by superposition and entanglement, which also gives the power of quantum computers and information processing. However, in addition to the two-state fermionic qubit, there is also another physical system, the bosonic one. In this case, any arbitrary non-negative number of bosonic particles is possible in a given state. It can also be in superposition and entangled state in the same way as its fermionic counterpart. The abstract unit here is *qumode*, which represents the number of particles in the given mode.

A quantum simulator operating on this principle is actually a sampling task called boson sampling [3]. In their famous paper, Aaronson and Arkhipov [1] proved that this is a classically hard-to-calculate problem. If we want to understand the simulator operating on such a principle more vividly, then the photonic probability quantum computer corresponds to a first approximation. As far as hardware implementation is concerned, tools for boson sampling have been used and developed in quantumoptics for decades. It consists of three major modules:

- bosonic particle source,
- simulation circuit,

- the detectors that measure the output.

There are several solutions for these modules. For example, we can use one-photon sources for the first module, quantumoptical elements – interferometers, phase shifters – in the middle one, and particle counters for the last one.

There is also a technically simpler and cheaper structure that uses coherent light instead of a single-photon source, i.e. a laser. A Gaussian distribution is used for the theoretical description of coherent light, so this type of quantum simulator is called Gaussian Boson Sampling [5]. Gaussian Boson Sampling is suitable for the implementation of new applications in addition to the modified version of existing algorithms. Calculating the vibrational spectra of molecules and their ions is also a very useful example in this kind of practice, since a deeper understanding of the spectroscopic properties enables, for example, the development of new biological markers or solar cell photocells.

The probability distribution of a given molecule or ion's electron emission or absorption process is called the Frank-Condon profile [6]. One method of calculating the Frank-Condon profile in the Born-Oppenheimer approximation is to describe the electrical energy surfaces of the states before and after the transition with quantum harmonic oscillators. The transition between these two quantum harmonic oscillators is described as an additional Duschinsky approximation with a linear transformation, the so-called Duschinsky mixing matrix.

With these approximations, the transformation between the eigenstates of harmonic oscillators can be described with the so-called Doktorov operator, and the square of the inner product of the eigenstates gives the transition probabilities. The Doktorov operator can be written as a product of linear quantum optical operators, namely the displacement, squeezing and rotation operators.

Quantumoptical devices perform these three transformations on coherent light. The middle module of boson sampling, the circuit that performs the rotation and phase shift, means performing the latter operation. Displacement and squeezing can be performed with other optical elements before the coherent light enters the circuit performing the simulation.

Hence the calculation of the Frank-Condon profile of molecules can be naturally implemented on a quantum simulator performing Gaussian Boson Sampling. Such measurements were physically performed for small molecules by Wang et al. [7] for four molecules, and by Huh et al. [4] for two molecules. The Frank-Condon factors obtained from each simulation agree with experimentally, spectroscopically measured data.

These boson sampling calculations can also be performed on quantum simulators running on a classical computer. Such a computation has been implemented in Xanadu's Strawberryfield simulator [8]. This work validated the data reported by Huh et al. for the formic acid and thymine molecules.

Another photonic quantum computer simulator, Piquasso [2], was developed in a cooperation with Eötvös Loránd University, Wigner Research Centre for Physics and Ericsson recently. This paper reports on a modified Gaussian Boson Sampling circuit developed on this platform, which not only reproduces successfully

the Frank-Condon profiles of the molecules in the paper of Huh et al., but also the results of Wang et al. To achieve this, it was necessary to introduce ancilla qumodes, as well as to define modified cutoffs for the finite capacity of classical computers. Going beyond the Frank-Condon profiles of molecules found in the articles of Huh et al. and Wang et al., the model developed in this way provides the possibility to calculate similar transition probabilities for additional molecules.

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