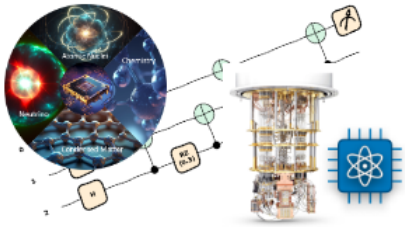

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Vibrational structure study: from qubit-based to photonic simulations

Friday, November 21, 2025 2:55 PM (25 minutes)

The vibrational structure is a challenging problem, which has been little explored compared to the electronic structure one [1,2]. For a qubit representation, one cannot directly map the bosonic states to two-level qubits [3]. Still, encodings of second-quantized bosonic operators to qubits have been determined previously [4,5]. If one can obtain a finite polynomial Taylor expansion of the potential, it is convenient to use a harmonic oscillator basis set for the analytic integrals of the position and momentum operators. Nevertheless, the latter basis set contains an infinite number of functions and must be truncated. Here, we highlight the crucial importance of the ordering of the second quantization bosonic operators, which is a consequence of the basis truncation. We illustrate the ordering effect on the spectrum of a system with a one-mode double-well potential using the aforementioned basis set. The model is chosen to describe a large-amplitude motion exhibiting fine splitting of its eigenvalues due to deep tunneling [6]. Another question at stake is: what is the optimal choice, for a simulation based on a quantum algorithm, of the origin of the basis for this prototypical Hamiltonian? To answer that, we compare the scaling of the 1-norm with respect to the number of qubits of the two Hamiltonians. We inspect as well the convergences of the low-lying eigenvalues and their corresponding eigenstates with respect to the number of basis functions. Because mapping bosonic states to qubits is either inefficient or leads to complex circuits, we then explore the representation and computation of bosonic systems using photonic operations. We focus on the vibrational spectrum of the stretching mode in the water molecule. To do so, we use an ansatz that is boson-number-preserving to work with polyads as done in the Harmonically Coupled Anharmonic Oscillators (HCAO) approximation [7]. To this end, we run the State Average Variational Quantum Eigensolver (SAVQE) to target all the eigenvalues in a polyad and show the importance of a physically inspired guess for the initial wave function with respect to different anharmonicity and mode-coupling regimes. We also implement a way to estimate the dipole-dipole term of the extended model in a noisy sampling scheme.

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