HamLib: A library of Hamiltonians for benchmarking quantum algorithms and hardware

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For a considerable time, large datasets containing problem instances have proven valuable for analyzing computer hardware, software, and algorithms. One notable example of the value of large datasets is ImageNet [1], a vast repository of images that has been instrumental in testing numerous deep learning packages. Similarly, in the domain of computational chemistry and materials science, the availability of extensive datasets such as the Protein Data Bank [2], the Materials Project [3], and QM9 [4] has greatly facilitated the evaluation of new algorithms and software approaches, while also promoting standardization within the field. These well-defined datasets and problem instances, in turn, serve as the foundation for creating benchmarking suites like MLPerf [5] and LINPACK [6], [7]. These suites enable fair and rigorous comparisons of different methodologies and solutions, fostering continuous advancements in various areas of computer science and beyond.

Though there has been progress in introducing benchmarks in the quantum computing community [8]–[13], there is not yet a broad database of problem instances covering many topics. Having such a dataset would be convenient for instance, when researchers wish to test a novel Hamiltonian simulation algorithm [14]–[17] for chemistry. Currently they must first go through the non-trivial process of preparing a set of chemical Hamiltonians on their own. It would be useful for the researcher to have these preparatory steps done ahead of time, so that they may spend more of their efforts on algorithm or hardware design.

The motivations behind creating a dataset of Hamiltonians with broad coverage in application area and in problem difficulty are the following: First, the existence of such a library can lead to significant time savings in labor. For instance, researchers aiming to evaluate their new quantum chemistry algorithms would be spared the burden of delving into the intricacies of electronic structure, installing and executing multiple packages, handpicking a suitable test set, and troubleshooting inevitable software issues. As a result, valuable resources and time can be redirected towards the more captivating aspects of algorithm and software development, fostering innovation and progress in these domains.

Second, a large Hamiltonian library enables more comprehensive testing capabilities. For instance, when conducting numerical tests on a novel Hamiltonian simulation algorithm, having immediate access to a diverse array of problems to run it on (rather than being limited to, say, a simple spin model and a handful of molecules) enhances the ability to gain a deeper understanding of the algorithm's performance under varying conditions.

Third, the existence of such a library facilitates reproducibility and standardization in research studies. When two algorithms are benchmarked using the exact same problem sets, it becomes much simpler to make fair and meaningful comparisons between them, ensuring a consistent and reliable basis for evaluating their performance.

To enable practical benchmarking of quantum algorithms, software, and hardware, we present a comprehensive dataset comprising numerous quantum *problem Hamiltonians* drawn from diverse fields like condensed matter physics, chemistry, and classical optimization. This dataset, named HamLib (Hamiltonian Library) version 1, aims to offer a wide array of Hamiltonians suitable for various applications. While our focus lies in providing this extensive collection of Hamiltonians, it is important to note that our primary goal does not revolve around defining specific benchmarks. The process of fully defining benchmarks, which typically involves not only identifying the problem and algorithm but also the dataset,

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falls outside the scope of this work.

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