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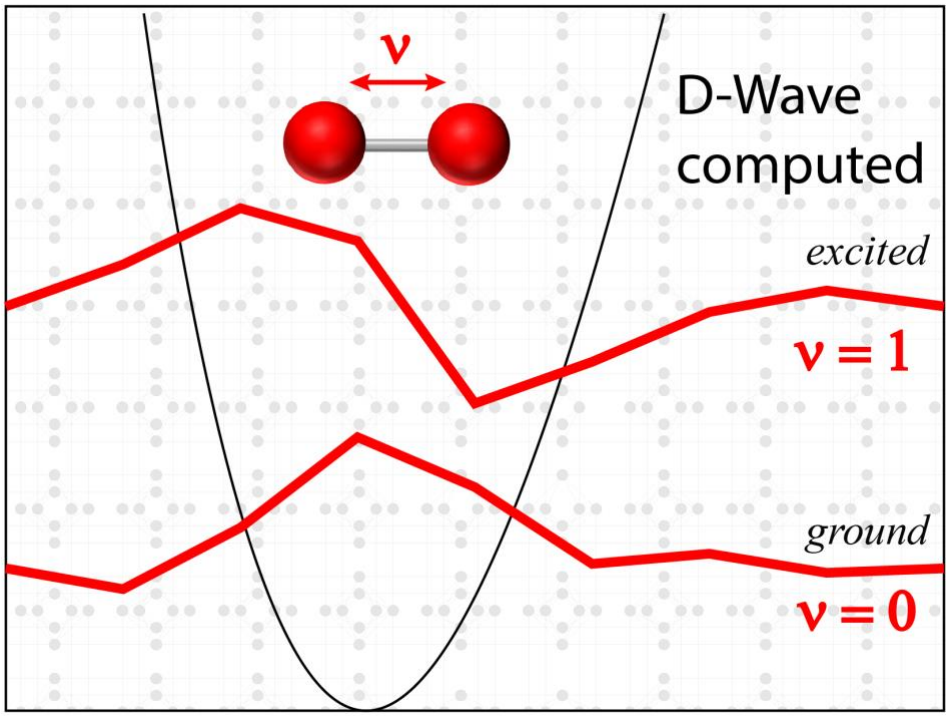
A Quantum Annealer Eigensolver (QAE) is Developed and Implemented on LANL's D-Wave Machine to Compute Molecular Vibrational Spectra

A Quantum Annealer Eigensolver (QAE) algorithm is developed to calculate the vibrational spectrum of a molecule on a quantum annealer. The method is demonstrated on LANL's D-Wave machine "Ising" to compute the lowest two vibrational states of O_2 (oxygen) and O_3 (ozone). The algorithm is general and represents a new revolutionary approach to solving the real symmetric eigenvalue problem on a quantum annealer.



The quantum annealer eigensolver (QAE) is developed and applied to compute the vibrational spectrum of a molecule on LANL's D-Wave machine "Ising". The D-Wave computed ground and first excited state vibrational wave functions of O_2 are plotted in red. The attractive interaction potential between the two oxygen atoms (red spheres) is plotted in black. The vibrational state is labeled by the quantum number ν where $\nu=0$ is the ground state and $\nu=1$ is the first excited state.

The Science

Until recently molecular energy calculations using quantum computing hardward have been limited to gate-based quantum computers. In this work, a new methodology is presented to calculate the vibrational spectrum of a molecule on a quantum annealer. The key idea of the method is a mapping of the ground state variational problem onto an Ising or quadratic unconstrained binary optimation (QUBO) problem by expressing the expansion coefficients for the molecular vibrational basis functions using spins or qubits. The algorithm is general and represents a new revolutionary approach for solving the real symmetric eigenvalue problem on a quantum annealer. The method is applied to two chemically important molecules: O_2 (oxygen) and and O_3 (ozone). Once the ground vibrational state is computed, spectral transformations are applied to compute the excited vibrational states. A key feature of the algorithm is the wave function normalization which is implemented by introducing an additional constraint to the QUBO functional. The weight multiplying the normalization constraint is optimized classically. The performance of the algorithm is quantified on both a hardware quantum annealer (LANL's D-Wave machine "Ising") and a software based classical annealer. Extension of the algorithm to higher dimensions is also explicitly demonstrated for an N-dimensional harmonic oscillator for $N \leq 5$. Noise simulations are performed which quantify the differences in performance between the hardware annealer (D-Wave machine) and noise-free classical software annealer.

The Impact

There are three key issues which limit practical applications using current generation NISQ (Noisy Intermediate Scale Quantum Devices): a) The small number of available qubits (which limits the problem size), (b) The large amount of noise present (which limits the accuracy), and (c) The lack of algorithms or techniques which map standard problems (such as the eigenvalue problem) onto the quantum hardware. Issues (a) and (b) are hardware technology issues which improve with each generation of quantum devices. Issue (c) is a theoretical challenge which is the focus of this work. Specifically, how does one map the standard variational eigenvalue problem which is prevalent throughout chemistry and physics onto a quantum annealer? The QAE algorithm developed and demonstrated in this work shows explicitly how to peform this mapping. The problem size and accuracy of the results based on QAE will continue to improve dramatically with the hardware improvements (a) and (b) discussed above.

Research Details

We used qbsolv as the software classical QUBO solver and the D-Wave 2000Q as the hardware quantum solver. The underlying qbsolv algorithm is a combination of Tabu search and a backbone-based method inspired by Glover, et al. The latter one is used for partitioning the original (large) QUBO into smaller sub-QUBOs. The only modification we did was to increase the span of partitioning to 1 (the hard-coded value is 0.214). The number of repeats in the stopping criterion is $N_{rep} = 10_4$. The hardware was accessed using qOp stack: qbsolv, DW library and SAPI. Although

qbsolv allows running sub-QUBOs on the hardware, we did not follow this approach, because the contribution of the D-Wave machine to the solution would be hard to estimate. Furthermore, qbsolv does implicit restarts and uses a classical Tabu search to refine solutions. Thus, a hardware calculation using the default qbsolv is actually hybrid and not fully quantum (for problems that fit one sub-QUBO qbsolv is completely classical). In order to bring the actual D-Wave performance to the surface, we removed partitioning, restarts and refinement from qbsolv, so that it only serves as an interface to the hardware. In addition, we raised the number of reads to 10_5 (the hard-coded value is 25). Our code generates input QUBO matrices for qbsolv. It is written in Fortran and uses LAPACK as the classical numerical eigensolver (for benchmarking the QUBO results).

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Publications

Calculation of Molecular Vibrational Spectra on a Quantum Annealer, J. Chem. Theory Comput. 2019, 15, 8, 4555-4563. DOI 10.1021/acs.jctc.9b00402. A. Teplukhin, B. K. Kendrick, and D. Babikov.

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