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Quantum computations of relativistic and many-body effects in atomic and molecular systems based on variational algorithms

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In this talk, I shall present results of our recent computations of relativistic and many-body effects in atomic and molecular systems on digital quantum computers and also the D-wave quantum annealer. The variational quantum eigensolver (VQE) was used to compute the hyperfine interaction constants for atomic systems and the dipole moments of molecular systems on superconducting and trapped ion platforms respectively. The ground-state energies were obtained as a byproduct of the calculations for both the cases and were determined to within one per cent of the classical computations. The corresponding errors for the hyperfine interaction constants and the molecular dipole moments were found to be larger. The interplay of relativistic and many-body effects for all the properties will be discussed.

Finally, the results for the fine-structure intervals in boron-like ions using the quantum annealer eigensolver (QAE) will be presented. This quantity is relativistic in origin, but is influenced by many-body effects. We have computed it to an accuracy of 99% on the D-wave annealer compared to high precision laboratory measurements. The reasons for achieving this high accuracy will be explained.

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