Abstract

Quantum computer can solve certain problems which are hard for conventional computer. Due to exponential size of Hilbert space it is intractable to simulate quantum systems on a conventional computer. Exact solution of Schrodinger equation within a finite one particle basis set full configuration interaction (FCI) is very computationally hard. Its complexity scales exponentially with a size of the system. In principle, quantum computers are capable to carry out such calculations with only polynomial scaling. Situation gets much harder when we consider solutions of relativistic molecular hamiltonians, so happens due to larger hamiltonian matrix eigen value problem and symmetry has also lost due to spin-orbit interaction which causes a significant large no. of integrals to be nonzero in Hamiltonian matrix. In this work, the simulation of molecular Hamiltonian of SbH molecule in CAS(2, 2) is discussed. The Hamiltonian matrix is obtained from DIRAC software in Kramer restricted approach and simulation involved implementation of adiabatic state preparation, iterative phase estimation which are discussed in detail. We used digital quantum simulation where controlled-U in phase estimation algorithm is decomposed into smaller unitary operators governed by local interaction Hamiltonian.