Title: Quantum computing algorithms for quantum chemistry

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Abstract: The topic of this study is the simulation of the quantum algorithm for the diagonalization of the matrix representation of the all-electron Dirac-Coulomb hamiltonian of the SbH molecule. Two different limited CI expansions were used to describe both the ground state ($X\ 0^+$) and the first excited doublet ($A\ 1$) by simulating the Iterative Phase Estinamtion Algorith (IPEA). In the simulations numerically performed in this work, the „compact mapping“ has been employed for the representation of the evolution operator $\exp(i\ \hat{H}\Delta t)$; in the theoretical part of the work, the „direct mapping“ is described as well. The influence of the metodics for choosing the initial eigenvector estimate is studied in both IPEA A and IPEA B variants. For those variants, the success probabilities p_m are computed for different single-points on the SbH dissociation curves. The initial eigenvector estimates based on the „CISD(2)“ method are found to be sufficient for both studied LCI-expansions up to internuclear distance $R \approx 6\ a_0$. The p_m dependence on the overlap between the eigenvector in question and its inital estimate - $\left|\langle\psi_0|\phi\rangle\right|^2$ is studied the for IPEA B method. The usability of the both variants of the IPEA in possible later calculations is disscused.