Title: Tensor-Factorized Hamiltonian Downfolding: Depth-Optimal Quantum Circuits for Many-Electron Wavefunction Emulation and Property Estimation

Abstract: Tensor-Factorized Hamiltonian Downfolding (TFHD) offers a tensorized eigenvalue-solver route to tackle strongly correlated, pharmaceutically relevant molecules on both classical and quantum hardware. By factorising the high-rank electronic integrals and wavefunction amplitude tensors that dominate post-Hartree–Fock theory into rank-two networks, TFHD reduces the formal scaling of full coupled-cluster treatments from N7 to N3 operations and N2 memory. GPU kernels built on this structure recover sub-milli-hartree accuracy for systems that include the 1 151-orbital FeMoCo cluster—an active-site size that would otherwise be out of reach for routine simulation.

The same rank-two description block-encodes naturally as a two-register quantum oracle requiring only logN logical qubits and a depth that grows quadratically with system size and only logarithmically with target precision. The solution from the eigensolver, i.e the many electron wavefunction is realized as a sparse shallow depth quantum circuit which can enable computation of multi-electron density matrices and quantum information theoretic measures with satisfiability properties on Quantum Computers, beyond 100 orbitals. The number slater determinant coefficients >10^75 and this cannot be stored on todays HPC's. However we position a quantum circuit realizable form of the many electron wavefunction that in turn enables constructing some of the higher order correlation properties relevant for Pharma use cases. TFHD therefore provides a unified, verifiable framework for advancing both high-accuracy quantum chemistry and early fault tolerant quantum computing.