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What Density Functional Theory could do for Quantum Information

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The Hohenberg-Kohn theorem of Density Functional Theory (DFT), and extensions thereof, tells us that all properties of a system of electrons can be determined through their density, which uniquely determines the many-body wave-function. Given access to the appropriate, universal, functionals of the density we would, in theory, be able to determine all observables of any electronic system, without explicit reference to the wave-function. On the other hand, the wave-function is at the core of Quantum Information (QI), with the wave-function of a set of qubits being the central computational resource in a quantum computer. While there is seemingly little overlap between DFT and QI, reliance upon observables form a key connection. Though the time-evolution of the wave-function and associated phase information is fundamental to quantum computation, the initial and final states of a quantum computer are characterized by observables of the system. While observables can be extracted directly from a system's wave-function, DFT tells us that we may be able to intuit a method for extracting them from its density. In this talk, I will review the fundamentals of DFT and how these principles connect to the world of QI. This will range from DFTs utility in the engineering of physical qubits, to the possibility of using it to efficiently (but approximately) simulate Hamiltonians at the logical level. The apparent paradox of describing algorithms based on the quantum mechanical many-body wave-function with a DFT-like theory based on observables will remain a focus throughout. The ultimate goal of this talk is to initiate a dialog about what DFT could do for QI, in theory and in practice.
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