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Nuclear Quantum Simulations on Quantum Computers in the Optimal Control Context

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One promising application of quantum computing consists in the simulation of quantum systems. The use of a device which is itself quantum should allow for a better management of the exponential scaling of time and memory resources needed to capture the details of quantum systems. Optimal control techniques provide a means to tailor control pulse sequences necessary for the generation of customized quantum gates implementing system's dynamics, moreover enhancing the resilience of quantum simulations to gate errors and device noise. However, the substantial amount of (classical) computing required for the generation of such customized gates can quickly spoil the effectiveness of this approach, especially when the pulse optimization needs to be iterated at every simulation time-step.
We propose a method to reduce the computing time required for the generation of these control pulses by the use of simple interpolation schemes to accurately reconstruct the control pulses starting from a batch of pulses obtained, in advance, for a discrete set of pre-determined values of the system's parameters. We then present device-level quantum simulations, carried out with this method, of two systems: the hydrogen atom in the hypothetical case in which the hydrogen Hamiltonian depends parametrically on a time-varying effective electron mass, and the scattering process of two neutrons whose spin dynamics depends instantaneously on their relative position. In both test cases, we obtain a high fidelity reconstruction and a substantial reduction of the computational effort showing how this method can help to improve quantum nuclear systems simulations on quantum devices.

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