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Quantum computing fidelity susceptibility using automatic differentiation

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Fidelity susceptibility is a physical quantity that can be used to study quantum phase transitions in a variety of condensed matter models. The closed-form expression of this quantity requires knowledge of the energy spectrum of a Hamiltonian; however it has been previously shown that it can also be computed from second-order derivatives of overlaps involving the ground state wave function. We show how such a calculation can be performed using variational quantum algorithms and quantum differentiable programming. Automatic differentiation is leveraged to compute the required energy and overlap derivatives directly from the results of quantum circuits, running on simulators or hardware, that have been trained to prepare the ground state of the system. We study a small case, using the transverse-field Ising model, and outline the viability and challenges that arise when solving this problem on near-term quantum hardware.

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