Efficient calculation of Green's functions on quantum computers via simultaneous circuit perturbation

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In this work, we focus on a new algorithm for the computation of the retarded Green's function (RGF) on quantum computers. We propose an efficient method (in the number of shots) to overcome the connectivity constraints of modern quantum devices that leverages randomized quantum circuit perturbations within a linear response-inspired framework.

Our solution is based on the representation of the generalized susceptibility as functional derivative: we show that the parameter-shift rule can be used to obtain an exact representation of the RGF, formalizing in this new context previous efforts [1] (local circuit perturbation, LCP).

We combine this idea with stochastic gradient estimation via simultaneous perturbation stochastic approximation (SPSA), to obtain a novel parallel-time algorithm to compute the target correlation functions. We refer to it as simultaneous circuit perturbation (SCP). We show how this approach not only bypasses circuit connectivity constraints, eliminating the need for long-range gates or swap overhead, but allows for a reduction in the number of circuit calls required to achieve a given variance of the RGF estimates. We test our method on both a Heisenberg spin chain and a 1D Fermi-Hubbard model.

References

[1] E. Kökcü, *et al.*, Nature Communications 15, 3881 (2024).

Figures

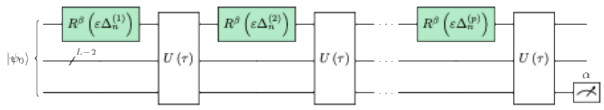

Figure 1: Circuit model for the proposed SCP protocol. Each rotation angle is an element sampled from a Rademacher distribution.

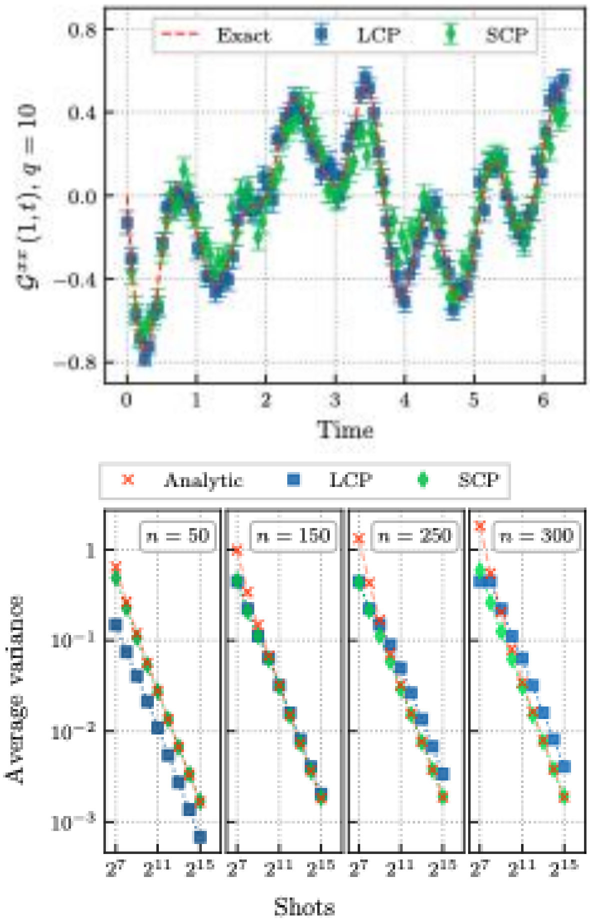

Figure 2: ***Top.*** Green's function for a 10-spin periodic Heisenberg chain. The expected Trotter dynamics is compared against the results produced with both LCP and SCP. ***Bottom.*** Average variance of the LCP and SCP methods as a function of the number of shots.