Computing Free Energies with Fluctuation Relations on Quantum Computers

Lindsay Bassman[1,*]
Katherine Klymko[1], Diyi Liu[2], Norman M. Tubman[3], Wibe A. de Jong[1]
[1]*Lawrence Berkeley National Lab, Berkeley, CA 94720*
[2]*Department of Mathematics, University of Minnesota, MN 55455*
[3]*NASA Ames Research Center, Mountain View, CA 94035*
*lbassman@lbl.gov

As a central thermodynamic property, free energy enables the calculation of virtually any equilibrium property of a physical system, allowing for the construction of phase diagrams and predictions about transport, chemical reactions, and biological processes [1]. Thus, methods for efficiently computing free energies, which in general is a difficult problem, are of great interest to broad areas of physics and the natural sciences. The majority of techniques for computing free energies target classical systems, leaving the computation of free energies in quantum systems less explored. Recently developed fluctuation relations enable the computation of free energy differences in quantum systems from an ensemble of dynamic simulations. While performing such simulations is exponentially hard on classical computers, quantum computers can efficiently simulate the dynamics of quantum systems [2]. Here, we present an algorithm utilizing a fluctuation relation known as the Jarzynski equality [3] to approximate free energy differences of quantum systems on a quantum computer. We discuss under which conditions our approximation becomes exact, and under which conditions it serves as a strict upper bound. Furthermore, we successfully demonstrate a proof-of-concept of our algorithm using the transverse field Ising model on a real quantum processor, see Figure 1. As quantum hardware continues to improve, we anticipate that our algorithm will enable computation of free energy differences for a wide range of quantum systems, providing a valuable tool for exploring thermodynamics in the quantum domain, where much remains to be discovered.

References

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Figures

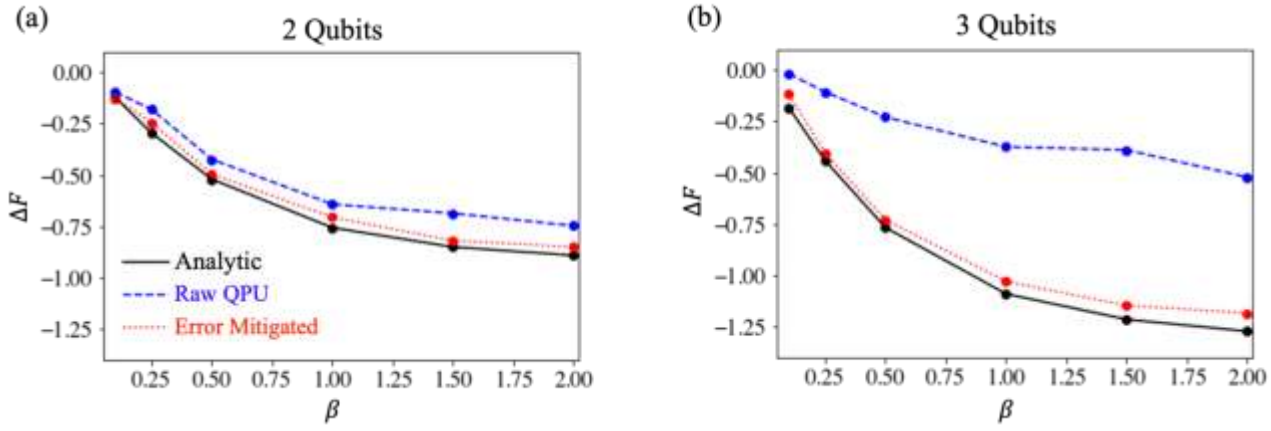

Figure 1: Approximate free energy differences for 2- and 3-qubit systems initialized at various inverse temperatures performed on an IBM quantum processing unit (QPU). The solid black line give the analytically computed values for reference. The blue dashed lines show raw results from the QPU, while the red dotted lines show these results after error mitigation has been performed.