Thermal States via Quantum Dynamical Emulation

Jacob Leamer^{1,2}, Denys I Bondar¹, and <u>Gerard McCaul</u>¹

¹Tulane University, 8208 plum street, New Orleans, USA ²Sandia National Laboratory

We introduce the concept of Quantum Dynamical Emulation, a constructive method for mapping the solutions of non-unitary dynamics to a weighted set of unitary operations. This allows us to derive a new correspondence between real and imaginary time, which we term Imaginary Time Quantum Dynamical Emulation (ITQDE). This enables an imaginary time evolution to be constructed from the overlaps of states evolved in opposite directions in real time. We show that a single trajectory evolved using ITQDE can be used not only to infer ground and thermal states, but also to resolve information about the complete Hamiltonian spectrum. We further employ ITQDE to derive novel thermodynamic results, including a generalisation of the Hubbard-Stratonovich transform. We go on to develop a quantum algorithm for computing the spectra of quantum systems that is based on this premise. We demonstrate the utility of this method through numerical simulation, as well as quantum hardware implementations.

This work was supported by both Sandia National Laboratories' Laboratory Directed Research and Development Program under Contract No. DE-NA0003525 as well as the Army Research Office (grant W911NF-23-1-0288; program manager Dr. James Joseph).