UNIVERSITY OF LOUISVILLE

COLLEGE OF ARTS & SCIENCES

Department of Chemistry

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Fewer Measurements from Shadow Tomography with N-Representability Conditions

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One of the most sought-after quantum computing applications is molecular simulation. However, obtaining a full description of an N-qubit quantum system requires an exponential number of measurements and classical memory, translating into very long quantum circuits on quantum hardware. Classical shadow tomography provides a randomized scheme for approximating the quantum state and its properties at reduced computational cost with direct applications in quantum computing. The output of this procedure is a classical shadow of an unknown quantum state that can be used to predict molecular properties. Here, we combine shadow tomography with additional physical constraints necessary for the measurements to be consistent with an N-electron quantum system. These constraints, known as N-representability conditions, significantly reduce the number of required measurements. We demonstrate the advantages of the algorithm by computing the ground- and excited-state properties of several molecular systems. The resulting tomography has the potential for significant applications in quantum many-body simulations on quantum devices.

Irma received her B.S. in Chemistry, graduating summa cum laude, from University of Louisville in May 2021. She subsequently attended the University of Chicago, where she obtained an M.S. in December 2022 and is now a Ph.D. candidate. While at University of Louisville, she completed an undergraduate honors thesis in the group of Lee Thompson, understanding how electric fields modify photoisomerization pathways of azobenzene derivatives, for which she was the recipient of the Best Natural Sciences Honors Thesis Award. She had three publications from her undergraduate work (including a first author paper) and received the ACS Outstanding Graduate in Chemistry Award. Since moving to the University of Chicago, her work in the group of David Mazziotti has been on developing and applying algorithms for molecular simulations on quantum computers. Her work has led to the publication of five articles, of which four are first author. During her graduate work she has been the recipient of a prestigious National Science Foundation graduate research fellowship, among other awards for mentoring, teaching and research.

References:

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