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OBJECTIVE

A theoretical position studying the fundamental role of information in physics.

STATEMENT

Expert in multi-disciplinary sciences (▼ quantum physics, ♥ biochemistry, ♦ information theory); algorithm development with ♣ classical and ■ quantum computers; communicating arcane concepts through teaching and writing; and in walking to unwalkable places.

EDUCATION

Ph.D - Physics

University of North Texas, Denton, TX exp. May 2022

MS - Physics

University of North Texas, Denton, TX Dec 2020

MS - Computer Science

Towson University, Towson, MD May 2017

BS cum laude - Physics; Molecular Biology, Biochemistry and Bioinformatics

Towson University, Towson, MD Aug 2015

PRESENTATIONS

▼ ◆ ■ - An adaptive pulse-level variational quantum eigensolver.
 Talk, APS March Meeting. 2024
 Poster, VTQ Symposium. 2023
 ▼ ▼ ● ■ - Julianic simulations of a pulse-level VQE.
 Talk, JuliaCon. 2023
 Talk, VTQ Internal Seminar. 2022

Talk, SCaN Breakout Intern Seminar. 2021 Talk, NASA/NRO Intern Symposium. 2021

Talk, SCaN Intern Symposium. 2021

Band theory on a quantum computer.
 Band theory and beyond.
 Poster, UNT MRS Poster Competition. 2022

Talk, Sandia National Labs. 2022

Talk, Lawrence Berkeley National Labs. 2022

Talk, Dartmouth College. 2022 Talk, Virginia Tech. 2022

Dissertation defense. 2022

Implementing Trans. Quantum Subspace Expansion with fewer qubits.
 Talk, APS March Meeting. 2022

Applying present-day quantum computers to materials science.
 Dissertation proposal. 2021

Band structure in a quantum computer.
 A tutorial in variational quantum computing.
 End-of-term presentation. 2019

Seeking complexity in a nonlinear equilibrium chemical potential.
 Student lecture. 2019

Predicting electron spin from scratch.
 Information reconciliation for erasure channels.
 End-of-term presentation. 2019
 Thesis defense. 2017

▼ ◆ ♣ - Information entropy of 1D quantum systems. Poster, *TU Research Expo.* 2015

- Surviving abroad without a smartphone. Poster, *TU Honors College Expo.* 2015

Exploring natural product formation with structural biology.
 Talk, MB3 Club Seminar, 2015

Poster, CTRC Summer Research Colloquium, 2014

- Computational simulation of electron diffraction.

Talk, HWI Weekly Seminar, 2014
- Poster, TU Research Expo. 2014

Poster, APS March Meeting. 2014

PUBLICATIONS

▼ ♥ ♦ ■ - On the scalability of pulse-level VQE with chemical complexity	(TBP)
▼ ♥ ◆ ■ - Avoiding symmetry roadblocks in pulse-level VQE	(TBP)
▼ ♥ ♦ ■ - An adaptive pulse-level variational quantum eigensolver	(TBP)
▼ ♥ ◆ ■ - Degrees of freedom in pulse-level VQE	(TBP)
 Quantum compressive sensing: mathematical machinery 	Appl. Sci. (12: 15). 2022
▼ ▼ ◆ ■ - Band theory and beyond: quantum algorithms for quantum chemistry	Poster and dissertation.* 2022
 Quantum algorithm for band structures with local tight-binding orbit 	als. Scientific Reports (12). 2022
A systematic band theory in a quantum computer.	RSC Adv. (11). 2021
Quantum computation of silicon band structure.	Phys. Chem. Chem. Phys. (22). 2020
 Seeking complexity in a nonlinear equilibrium chemical potential. 	Report.* 2019
 Music theory: methods for mathematical music. 	Report.* 2018
Hello, World!—Code Responsibly.	IEEE Security & Privacy (16: 1). 2018
 Information reconciliation for erasure channels. 	Master's thesis.* 2017
Information entropy of 1D quantum systems.	Poster and report.* 2015
 Surviving abroad without a smartphone. 	Poster.* 2015
 An analysis of the PLAST model for quasars. 	Term paper.* 2014
 - The Circus Game. 	Pedagogical short story.* 2014
 Scarlet's Letters. 	Pedagogical short story.* 2014
 Exploring natural product formation with structural biology. 	Poster and report.* 2014

^{*} Available on my personal website, kmsherbert.neocities.org

- Computational simulation of electron diffraction.

RESEARCH EXPERIENCE

Post-doctoral Researcher Fall 2022-Present

Departments of Chemistry, Physics, Virginia Tech, Blacksburg, VA Faculty Mentors: Nick Mayhall, Sophia Economou, Ed Barnes

- Explored alternative pool choices for sc-ADAPT-VQE in characterizing the Schwinger model.
- 🔻 🖤 🔸 🔳 Adapted the ADAPT-VQE algorithm to use Renyi divergence as a cost function.
- ▼ ♥ ♣■- Assisted in the development of a dedicated Julia package representing Pauli operators.
- 🔻 🗣 🔹 Supported fellow postdoc in applying the BKSF qubit mapping to ADAPT-VQE
- ▼ ▼ - Supervised graduate student in implementing ctrl-VQE in available quantum hardware.
- Developed novel adaptive algorithm to strategically add in parameters in ctrl-VQE.
- ▼ - Derived symmetry no-go conditions when starting ctrl-VQE from an inert pulse.
- ▼ ■ Characterized impact of frequency and phase degrees of freedom on ctrl-VQE.
- 🔻 🗣 👢 Implemented optimized Julia code to simulate ctrl-VQE experiments.
 - **Presented work** at APS March Meeting, JuliaCon, and VTQ Symposium.

Doctoral Dissertation Fall 2019-Spring 2022

Department of Physics, University of North Texas, Denton, TX

Faculty Mentor: Marco Buongiorno Nardelli

- Adapted quantum algorithms for quantum chemistry to solve problems in materials science (band structures) and information theory (compressive sensing).
- Developed novel strategy to locate excited states in variational quantum algorithms.
 - Developed quantum circuits and protocols for compressive sensing in a quantum computer.
- Developed three distinct quantum algorithms for band structure calculations using qiskit, cirq.
- Validated quantum algorithm using IBMQ Experience quantum computers.
- ▼ - Derived statistical error for quantum variational excitation algorithm.
 - Presented work at UNT MRS Poster Competition and numerous academic seminars.

Virtual Intern Summer 2021-Spring 2022

NASA Goddard Space Flight Center, Greenbelt, MD

Mentor: Harry Shaw

- Simulated molecular candidates for quantum oscillator in GAMESS.
- Designed quantum compressive sensing protocol for LIDAR imaging with Born machines.
- • Implemented classical approximation to quantum compressive sensing protocol using tensor networks in Python.
- Developed quantum circuits and protocols for compressive sensing in a quantum computer.

Poster.* 2014

- **Presented work** in VTQ Internal Seminar and multiple NASA seminars.
- Published article in Appl. Sci. (12).

Research Assistant Fall 2019-Spring 2022

Department of Physics, University of North Texas, Denton, TX

Faculty Mentor: Marco Buongiorno-Nardelli

- - Developed novel strategy to locate excited states with variational quantum algorithms.
- Developed systematic quantum algorithm for band structure calculations using qiskit, cirq.
 - - Validated quantum algorithm using IBMQ Experience quantum computers.
- Calculated band structure of silicon with variational quantum eigensolver.
 - Derived statistical error for quantum variational excitation algorithm.
 - Presented work at APS March Meeting 2021, 2022 and ES22 Invited Talk.
 - Published articles in Scientific Reports (12), RSC Adv. (11) and Phys. Chem. Chem. Phys. (22).

Research Assistant Spring 2019

Department of Physics, University of North Texas, Denton, TX

Faculty Mentor: Paolo Grigolini

- Modeled and simulated non-linear Langevin dynamics of model enzyme reaction using Python.
 - Studied temporal complexity by approximating reaction wait-time distribution using stochastic calculus.
 - Presented work in student lecture for PHYS 6500.

Research Assistant Fall 2018

Department of Physics, University of North Texas, Denton, TX

Faculty Mentor: Marco Buongiorno-Nardelli

- Investigated metamolecular dynamics of small Lennard-Jones clusters using Python.
 - - Surveyed existing libraries for developing quantum algorithms.
- Verified validity of Fourier differentiation in PAOFLOW electronic structure software.

Master's Thesis Fall 2016-Spring 2017

Department of Computer and Information Sciences, Towson University, Towson, MD

Faculty Mentor: Marius Zimand

- Reviewed literature on Slepian-Wolf coding, information erasure reconciliation.
- • Simulated information erasure reconciliation using various protocols using Python.
- • Proposed novel probabilistic protocol for reconciling erasures.
- Measured protocol's empirical error-rate and optimal communication efficiency.
- Approximated theoretical error-rate and optimal communication efficiency.

Graduate Assistant Fall 2015-Spring 2017

Department of Computer and Information Sciences, Towson University, Towson, MD Faculty Mentors: Siddharth Kaza, Blair Taylor

- - Created Data Hiding module for Security Injections repository.
- Designed and supervised development of Security Injections 3.0.
- Maintained web resources for Towson University's Cyber4All initiative.
 - Wrote NSF Grant Report assessing progress and project outlook.
 - **Published article** in *IEEE Security and Privacy* article.

Research Assistant Spring 2015

Dept. of Physics, Astronomy, and Geosciences, Towson University, Towson, MD

Faculty Mentor: Jia-An Yan

- Studied information entropy of scattering quantum systems using Matlab.
 - Analytically solved information entropy of free particle as a function of time.
- Replicated Phys. Rev. Lett. work studying fractional revivals in bound quantum systems.
 - **Presented work** at 2015 Towson University Research Expo.

Research Intern Summer 2014

Univeristy at Buffalo, Hauptman-Woodward Medical Research Institute, Buffalo, NY

Principal Investigator: Andrew Gulick

- Laboratory Mentor: Geoffrey Lippa
 - Performed site-directed mutagensis to introduce point mutations in *E. coli* plasmid.
- Mutated, expressed, and purified a bacterial enzyme for crystallization.

- Conjectured reaction pathway based on product/byproduct elution patterns.
- Proposed deletion experiment based on predicted structure to test conjecture.
 - Presented work at HWI Weekly Seminar, CTRC Summer Research Colloquium, and MB3 Club Seminar.

Winter 2014 **Capstone Project**

Dept. of Physics, Astronomy, and Geosciences, Towson University, Towson, MD

Faculty Mentor: Jia-An Yan

- Numerically solved Schrödinger's wave equation for a diffracting electron using Matlab.
 - Calculated reflection and transmission coefficients from energy transformation.
- Compared optical Talbot effect with electron-beam analogue.
 - **Presented work** at APS March Meeting 2014 and TU Research Expo.

TEACHING EXPERIENCE

▼

Instructor Summer 2024

Brookhaven National Laboratory, Yaphank, NY

- - Adapted curriculum for quantum information and quantum computing using a pictoral formalism.
- - Delivered lectures, activities, and assignments for intensive and engaging one-week summer course.
 - Mentored a graduate student in developing communication and organization skills.

Instructor Summers 2022-2023

Center for Talented Youth, Johns Hopkins University

- Developed curriculum for intensive summer courses for many subjects: Data Structures and Algorithms, Cryptography, Special Relativity.
 - Delivered lectures, activities, and assignments for intensive and engaging three-week summer course.
 - Mentored a teaching assistant in developing communication and organization skills.
 - Tracked student progress in content, critical thinking, and engagement, for end-of-session evaluations.

Online Instructor Summer 2020-Spring 2022

Center for Talented Youth, Johns Hopkins University

- Guided students through asynchronous Programming in Python for Middle-school Students online course.
- Tutored students all around the globe one-on-one in programming concepts and Python syntax.
- Executed, debugged, graded, and provided feedback on programming assignments.
 - Tracked student progress in content, critical thinking, and engagement, for end-of-course evaluations.

Teaching Assistant Fall 2018-Spring 2020

Department of Physics, University of North Texas, Denton, TX

- Assisted lecturer in *Musical Acoustics* course with 100+ students.
 - Laboriously graded daily quizzes and quarterly exams.
 - Learned every student's name so they knew they were loved.
 - Adapted course format to online learning when global pandemic struck mid-semester.
- Facilitated labs for General Physics I.
- Supervised students in *Computational Physics* and provided guidance as needed.

Teaching Assistant Summers 2015-2019

Center for Talented Youth, Johns Hopkins University

- Assisted instructor in intensive summer courses for middle- and high-schoolers over many subjects: Astrophysics, Fundamentals of Computer Science, Cryptography, Data Structures and Algorithms, Genomics, Investigations in Engineering.
- - Organized "lunchtime lessons" for introducing students to non-curricular scientific topics of interest.
 - Tracked student progress in content, critical thinking, and engagement, for end-of-session evaluations.

Substitute Teacher Spring 2018

Archdiocese of Washington

Schools: St. Mary of the Assumption Catholic School, Cardinal Hickey Academy

- Taught Pre-K to 8th grade, all grades and all subjects, over four months.
 - Awakened Kindergarten students to world geography following the story of Jonah.
- Designed curriculum for three-day stint as SMA middle-school math and science teacher.

- Substituted long-term for Spanish, all grades, at CHA.

Graduate Assistant Fall 2018-Spring 2020

Department of Computer and Information Sciences, Towson University, Towson, MD

- Assisted lecturer in *General Computer Science* and *Introduction to Computer Science I* courses.
- - Supervised students in lab and provided guidance as needed.
- Executed, debugged, graded, and provided feedback on programming assignments.
- Tutored online high-school students enrolled in SPLASH program.

Grader Spring 2014

Dept. of Physics, Astronomy, and Geosciences, Towson University, Towson, MD

- Graded homeworks for *Introductory Mathematical Physics*.
- Traced students' mistakes and provided consistent feedback.

ADDITIONAL EXPERIENCE

Church Choir - Accompanist

2011-Present

- Accompanied choir on clarinet, piano for weekly Catholic Mass.

Denton Community Band, Blacksburg Community Band - Clarinetist

2018-Present

- Played clarinet in an ensemble for seasonal concerts and Santa Serenades.

Christian Graduate Fellowship - President

2018-2022

University of North Texas, Denton, TX

- Organized weekly bible study and community night.

Senior Software Developer

Fall 2017

 $Department\ of\ Computer\ and\ Information\ Sciences,\ Towson\ University,\ Towson,\ MD$

Supervisor: Siddharth Kaza

- Designed database for CLARK cybersecurity curriculum management system using MongoDB, Angular.
- Developed CLARK microservice to suggest and search for learning outcomes.

Society of Physics Students

2012-2016

Dept. of Physics, Astronomy, and Geosciences, Towson University, Towson, MD

- Taught physics to young (age 6-10) students in Hampden Family Center.
- Demoed "Shoot the Monkey" station at 2016 Physics of Superheroes! event.
- Magician's assistant in 2013 *Physics is Magic!* Saturday Science show.

College Scholarship Committee - Student Representative

2015

Jess and Mildred Fisher College of Science and Mathematics, Towson University, Towson, MD

- Selected 2015 recipients of Jess Fisher FCSM and Pre-Engineering Scholarships.

Honors College Leadership Council

2012-2014

Honors College, Towson University, Towson, MD

- Organized college-prep event hosting AVID middle-schoolers at Honors College.
- Organized "Sweets, Stars, and Structure of the Universe" planetarium event.
- Redesigned Honors College Community page on Blackboard Learn.

AWARDS

U.S. Department of Energy Grant: DE-SC0019432 (Research Assistantship)	2019-2022
UNT College of Science Travel Award	2020
Maryland Space Grant Consortium Scholar	2014-2015
Edward L. Rubendall Outstanding Physics Student	2012-2014
Jess Fisher FCSM Scholar (Full Tuition)	2011-2015
Maryland Distinguished Scholar	2011-2015
Towson University Honors Scholar	2011-2015

COMPUTER SKILLS

Languages: Julia, Python (Anaconda), Java, JavaScript (Angular), Perl, Matlab, C/C++/C#

Quantum: Cirq (Google), Qiskit (IBMQ Experience), PyQuil (Rigetti Computing)

Chemistry: GAMESS, MacMolPlt Other: Unix, LaTeX, Git, HTML5, CSS3