Omar A. Ashour

Postdoctoral Researcher, Berkeley Lab

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Theoretical physicist specializing in interpretable AI, working at the intersection of deep learning, statistical mechanics, and mathematical physics. Research encompasses mechanistic interpretability of deep neural nets and development of physically-informed generative models for materials science and structural biology.

Education

University of California, Berkeley 2019 – 2025
PhD, Theoretical and Computational Physics *Advisor:* Sinéad Griffin
MA, Physics
Dissertation: Dark Matter Couture: Designer Targets and Tailored Detectors for Next-Generation Searches

University of California, Berkeley 2017 – 2019
MS, Applied Science (College of Engineering)
Thesis: The Nonlinear Schrödinger Hierarchy: from Quasi Rogue Waves to Nonlinear Talbot Carpets

Texas A&M University 2013 – 2017
BS, Electrical Engineering (*Summa Cum Laude*)
Thesis: Maximal Intensity Higher-Order Breathers of the Nonlinear Schrödinger Equation

Professional Experience

Postdoctoral Researcher Lawrence Berkeley National Lab
Computing Sciences Area and Molecular Foundry 07/25 – Present

- Developing physics-inspired analytical frameworks for mechanistic interpretability.
- Validating these techniques on real models, ranging from small neural nets to state-of-the-art language models.
- Building physically interpretable generative models for materials science and structural biology.

Quantum Computing PhD Intern NERSC
In collaboration with NASA and QuEra 05/24 – 08/24

- Designed an alternative loss function for a standard quantum algorithm— $\mathcal{O}(N^2)$ vs. $\mathcal{O}(N^4)$ measurements.
- Implemented loss function in a circuit simulator and ran $\mathcal{O}(10^6)$ numerical experiments on molecules.
- Identified chemical systems where the new algorithm's accuracy is comparable to original implementation.

Selected Software Packages

DarkMAGIC [Python with MPI/Numba]
Parallel, high-throughput package for calculating dark matter interactions with materials.

`pymatgen.io.espresso` [Python]
Infrastructure package democratizing the standard computational materials science stack.

Quesadilla [Python/Fortran]
Drop-in replacement for the community standard package for phonon calculations, but with linear (vs cubic) scaling.

Selected Research Projects

Quantum Materials for Dark Matter Detection and Quantum Sensing

- Devised novel approaches for dark matter detection employing new tools from condensed matter physics.
- Developed several analytical techniques and computational implementations to validate my approach.
- Served as a bridge between materials scientists, particle physicists, and stakeholders.
- Mentored two students who received funding to develop experimental implementations of my theoretical proposals.

Efficient Solvers for Nonlinear Schrödinger-type PDEs in Julia [arXiv]

- Independently conceived and developed the Julia package `NonlinearSchrodinger.jl` from the ground up.
- Fine-tuned 32 numerical algorithms that optimize performance within this specialized problem domain.
- Devised the first open-source numerical implementation of the analytical Darboux Transformation method.
- Implemented a simple API and data visualization tools enabling calculation of PDE solutions with a few lines of code.

Selected Fellowships and Awards

Finalist for the **University of California President's Postdoctoral Fellowship**	2025
Elected to full membership of **Sigma Xi**	2025
Ovshinsky Travel Award, American Physical Society, Division of Materials Physics	2024
Berkeley Graduate Fellowship, University of California, Berkeley	2017 – 2019
Anselmo J. Macchi Graduate Fellowship, University of California, Berkeley	2018 – 2019
Richard E. Ewing Award for excellence in student research, Texas A&M Univeristy	2016

Skills and Tools

Programming	Python; Julia; FORTRAN; MATLAB; C/C++.
Python Stack	NumPy; Numba; MPI4Py; SciPy; Pandas; Gudhi; PyTorch.
Numerics	ODEs; Nonlinear, coupled, and diffusion PDEs; SDEs; Topological data analysis.
Math	PDEs; Diff. geometry; Group/representation theory; Lie theory; Algebraic topology.
HPC	MPI, OpenMP, OpenACC. 12 years of experience with clusters.
Misc.	Git; CI/CD; Docker; Kubernetes; Basic webdev (Flask, PostgreSQL, MongoDB, JS).

Tangent Bundle

Gardening: I maintain a digital garden for research and pedagogy at `https://ashour.dev`.

4x MVP: I was voted *Most Valuable Physicist* by my research group (2021–2024) for community building.

Languages: English (bilingual), Arabic (bilingual), Spanish/French/German (abysmal).

Hobbies: I build mechanical keyboards and enjoy reading (currently geopolitics, spy thrillers, and sci-fi).

Erdös–McDonald's number: 19 (= Erdös number + # of countries where I've tried McDonald's).

Addendum: Selected Publications

⋆ Equal Contribution † Corresponding Author

2025 Guy C. Moore, Matthew K. Horton, Aaron D. Kaplan, **Omar A. Ashour**, Sinéad M. Griffin, and Kristin A. Persson. Noncollinear ground states of solids with a source-free XC functional, *Phys. Rev. B*, **111**, 094417 (2025).

2025 Thomas F. Harrelson, Ibrahim Hajar, **Omar A. Ashour**, and Sinéad M. Griffin. Theoretical investigation of decoherence channels in athermal phonon sensors, *J. Phys. Condens. Matter*, **37**, 015002 (2025).

2024 Nicholas Dale⋆, **Omar A. Ashour**⋆, Marc Vila, Justin Fox, Resham Regmi, Alexei Fedorov, Alexander Stibor, Nirmal Ghimire, and Sinéad M. Griffin. Non-relativistic spin splitting above and below the fermi level in a *g*-wave altermagnet (2024). [arXiv:2411.18761] *(Under Review at Nature)*

2024 **Omar A. Ashour**† and Sinéad M. Griffin. Pressure-tunable targets for light dark matter direct detection: the case of solid helium (2024). [arXiv:2409.02439] *(Under Review at Phys. Rev. Letters)*

2024 Na Hyun Jo⋆, **Omar A. Ashour**⋆, Zhixue Shu, Chris Jozwiak, Aaron Bostwick, Sae Hee Ryu, Kai Sun, Tai Kong, Sinéad M. Griffin, and Eli Rotenberg. Effects of strain, defects, and interactions on the topological properties of $HfTe_5$, *Phys. Rev. B*, **109**, 235122 (2024), ***Editor's Suggestion***.

2022 Stanko N. Nikolić, Sarah Alwashahi, **Omar A. Ashour**, Siu A. Chin, Najdan B. Aleksić, and Milivoj R. Belić. Multi-elliptic rogue wave clusters of the nonlinear Schrödinger equation on different backgrounds, *Nonlinear Dynamics*, **108**, 479–490 (2022).

2022 **Omar A. Ashour**†, Siu A. Chin, Stanko N. Nikolić, and Milivoj R. Belić. Higher-order breathers as quasi-rogue waves on a periodic background, *Nonlinear Dynamics*, **107**, 3819–3832 (2022).

2022 Thais Chagas⋆, **Omar A. Ashour**⋆, Guilherme Ribeiro, Wendell Silva, Zhenglu Li, Rogério Magalhães-Paniago, Yves Petroff, and Steven G. Louie. Multiple strong topological gaps and hexagonal warping in Bi_4Te_3, *Physical Review B*, **105**, L081409 (2022).

2022 Milivoj R. Belić, Stanko N. Nikolić, **Omar A. Ashour**, and Najdan B. Aleksić. On different aspects of the optical rogue waves nature, *Nonlinear Dynamics*, **108**, 1655–1670 (2022).

2021 **Omar A. Ashour**†. NonlinearSchrodinger: higher-order algorithms and Darboux transformations for nonlinear Schrödinger equations (2021). [arXiv:2103.14469]

2019 Stanko N. Nikolić, **Omar A. Ashour**, Najdan B. Aleksić, Yiqi Zhang, Milivoj R. Belić, and Siu A. Chin. Talbot carpets by rogue waves of extended nonlinear Schrödinger equations, *Nonlinear Dynamics*, **97**, 1215–1225 (2019).

2019 Stanko N. Nikolić, **Omar A. Ashour**, Najdan B. Aleksić, Milivoj R. Belić, and Siu A. Chin. Breathers, solitons and rogue waves of the quintic nonlinear Schrödinger equation on various backgrounds, *Nonlinear Dynamics*, **95**, 2855–2865 (2019).

2017 Stanko N. Nikolić, Najdan B. Aleksić, **Omar A. Ashour**, Milivoj R. Belić, and Siu A. Chin. Systematic generation of higher-order solitons and breathers of the Hirota equation on different backgrounds, *Nonlinear Dynamics*, **89**, 1637–1649 (2017).

2017 Runze Li, **Omar A. Ashour**, Jie Chen, H. E. Elsayed-Ali, and Peter M. Rentzepis. Femtosecond laser induced structural dynamics and melting of Cu (111) single crystal: an ultrafast time-resolved x-ray diffraction study, *Journal of Applied Physics*, **121**, 055102 (2017).

2017 Siu A. Chin, **Omar A. Ashour**, Stanko N. Nikolić, and Milivoj R. Belić. Peak-height formula for higher-order breathers of the nonlinear Schrödinger equation on non-uniform backgrounds, *Physical Review E*, **95**, 012211 (2017).

2016 Siu A. Chin, **Omar A. Ashour**, Stanko N. Nikolić, and Milivoj R. Belić. Maximal intensity higher-order Akhmediev breathers of the nonlinear Schrödinger equation and their systematic generation, *Physics Letters A*, **380**, 3625–3629 (2016).

2015 Siu A. Chin, **Omar A. Ashour**, and Milivoj R. Belić. Anatomy of the Akhmediev breather: cascading instability, first formation time, and Fermi-Pasta-Ulam recurrence, *Physical Review E*, **92**, 063202 (2015).