

Xuanzhao Gao

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EDUCATION

Hong Kong University of Science and Technology, Hong Kong SAR, China

2021 -- now

P.h.D. in Individual Interdisciplinary Program (Advanced Materials), supervised by [Prof. Zecheng Gan](#)

The University of Science and Technology of China, China

2017 -- 2021

B.S. in Condensed Matter Physics

RESEARCH INTERESTS

I am interested in applied and computational mathematics in general, with a particular focus on developing efficient numerical algorithms for modeling and simulating complex systems. Specifically, I am engaged in research on fast summation algorithms tailored for long-range interactions. I have also concentrated on algorithms for combinatorial optimization problems.

PUBLICATIONS

- [1] X. Gao, Q. Zhou, Z. Gan, and J. Liang, Accurate error estimates and optimal parameter selection in Ewald summation for dielectrically confined Coulomb systems, Arxiv Preprint Arxiv:2503.18126 (2025), accepted by Journal of Chemical Theory and Computation
- [2] Z. Gan, X. Gao, J. Liang, and Z. Xu, Random batch Ewald method for dielectrically confined Coulomb systems, Arxiv Preprint Arxiv:2405.06333 (2025), accepted by SIAM Journal on Scientific Computing
- [3] X. Gao, X. Li, and J. Liu, Programming guide for solving constraint satisfaction problems with tensor networks, Chinese Physics B (2025)
- [4] X. Gao, Y.-J. Wang, P. Zhang, and J.-G. Liu, Automated discovery of branching rules with optimal complexity for the maximum independent set problem, Arxiv Preprint Arxiv:2412.07685 (2024)
- [5] X. Gao, S. Jiang, J. Liang, Z. Xu, and Q. Zhou, A fast spectral sum-of-Gaussians method for electrostatic summation in quasi-2D systems, Arxiv Preprint Arxiv:2412.04595 (2024)
- [6] Z. Gan, X. Gao, J. Liang, and Z. Xu, Fast algorithm for quasi-2D Coulomb systems, Journal of Computational Physics **524**, 113733 (2025)
- [7] M. Roa-Villescas, X. Gao, S. Stuijk, H. Corporaal, and J.-G. Liu, Probabilistic inference in the era of tensor networks and differential programming, Physical Review Research **6**, 33261 (2024)
- [8] X. Gao and Z. Gan, Broken symmetries in quasi-2D charged systems via negative dielectric confinement, The Journal of Chemical Physics **161**, (2024)
- [9] Z. Nie, X. Gao, Y. Ren, S. Xia, Y. Wang, Y. Shi, J. Zhao, and Y. Wang, Harnessing hot phonon bottleneck in metal halide perovskite nanocrystals via interfacial electron-phonon coupling, Nano Letters **20**, 4610 (2020)

PRESENTATIONS AND POSTERS

SciCADE 2024, Contributed Talk

July 15-19, 2024

Fast Algorithm for Quasi-2D Coulomb Systems

ICIAM 2023, Poster

August 20-25, 2023

Random Batch Quasi-Ewald Method for the Simulations of Charged Particles under Dielectric Confinement

SKILLS

Programming Languages: Julia (proficient), Python, C/C++

Languages: Mandarin Chinese (native), English (proficient)