

Lei Wang

Curriculum Vitae

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Personal data

Day of Birth	1st December 1983	Nationality	China
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Academic Positions

2019.9– Present **Professor**, *Institute of Physics, Chinese Academy of Sciences*, Beijing, China.

2016.3– 2019.8 **Assistant Professor**, *Institute of Physics, Chinese Academy of Sciences*, Beijing, China.

2015.6 – 2016.2 **Senior research assistant (Oberassistent I)**, *ETH*, Zurich, Switzerland.

2011.9 – 2015.5 **Postdoctoral research assistant**, *ETH*, Zurich, Switzerland.
Supervisor: Prof. Dr. Matthias Troyer

Education

2006.9– 2011.7 **PhD in Physics**, *Institute of Physics, Chinese Academy of Sciences*, Beijing, China.
Supervisors: Prof. Xincheng Xie and Prof. Xi Dai

2002.9– 2006.6 **BSc in Physics**, *Nanjing University*, Nanjing, China.

Interests

AI Deep learning and its application in scientific discoveries
Computation New algorithms for quantum many-body computation
Physics Emergence and universal laws in many-body systems

Organized events

August 2016 **International Summer School on Computational Approaches for Quantum Many Body Systems**, *University of Chinese Academy of Sciences*, Beijing, China.

July 2017 **Machine Learning and Many-Body Physics School and Conference**, *Kavli Institute for Theoretical Sciences*, Beijing, China.

July 2018 **Conference on Machine Learning and Physics**, *Tsinghua University*, Beijing, China.

May 2019 **Spring School on Deep Learning and Quantum Programming**, *South Bay Interdisciplinary Science Center*, Dongguan, China.

- August 2022 **The 3rd Conference on Mathematical and Scientific Machine Learning**, Peking University, Beijing, China.
- November 2024 **Artificial Intelligence for Theoretical Sciences**, IOP, Beijing, China.

Selected Talks

- Feb 2013 **Simulating dynamics and topological phases of cold fermionic gases**, *Finite-temperature non-equilibrium superfluid systems*, Queenstown, New Zealand.
- June 2013 **Topological charge pumping of cold atoms**, *Topological Phases in Condensed Matter and Cold Atom Systems: towards quantum computations*, Cargese, France.
- Feb 2015 **Surprises in simulation of quantum phase transitions**, *Workshop on Quantum Simulations*, Benasque, Spain.
- April 2016 **New Adventures in Quantum Monte Carlo Method - How Did I Earn an Erdős Number of Two?**, *The 6th Workshop on Quantum Many-Body Computation*, Beijing Computational Science Research Center, China.
- March 2017 **Can Machine Learning Teach Us Cluster Updates ?**, *SIGN 2017: International Workshop on the Sign Problem in QCD and Beyond*, INT Seattle, USA.
- July 2017 **Machine Learning for Many-body Physics**, *Planetary Talk at Fourth National Conference on Statistical Physics and Complex Systems*, Xiaan, China.
- September 2017 **Artificial Intelligence and Quantum Physics**, *Public lecture at AI in Physics Salon*, Beijing Computational Science Research Center, China.
- March 2018 **From Boltzmann Machines to Born Machines**, *Invited Talk at APS March Meeting*, Los Angeles, USA.
- Sep 2018 **Neural Network Renormalization Group**, *Invited Talk at Physical Society of Japan Autumn Meeting*, Kyotanabe, Japan.
- Dec 2018 **Tensor Networks for Generative Modeling**, *Tensor Network States: Algorithms and Applications*, RIKEN R-CCS, Japan.
- July 2019 **Differentiable Programming Tensor Networks and Quantum Circuits**, *Machine Learning for Quantum Design*, Perimeter Institute, Canada.
- Feb 2021 **Neural Canonical Transformations**, *Quantum Cafe Webinar*, CCQ Flatiron Institute, USA.
- August 2021 **Fermi Flow: Ab initio study of fermions at finite temperature**, *Invited Presentation at XXXII IUPAP Conference on Computational Physics*, Coventry, England.
- March 2022 **m^* of electron gases: a neural canonical transformation study**, *Invited Talk at APS March Meeting*, Chigago, USA.
- Sep 2023 **Unlocking the Power of the Variational Free-Energy Principle with Deep Generative Models**, *Statistical Physics and Machine Learning*, Leipzig, Germany.
- June 2023 **A deep variational free energy approach to dense hydrogen**, *Machine Learning for Quantum Many-Body Systems*, Perimeter Institute, Canada.
- March 2024 **CrystalFormer**, *SQAI-NCTS Workshop on Tensor Network and Quantum Embedding*, Tokyo, Japan.
- December 2025 **Neural Canonical Transformations**, *Fermionic Neural Quantum States Workshop*, Paris, France.

Lectures

- Feb 2018 **Deep Learning and Quantum Many-Body Computation**, *FOR 1807 Winter School on Numerical Methods for Strongly Correlated Quantum Systems*, Marburg, Germany.
- October 2018 **Generative Models for Physicists**, *School and Conference on Physics, Inference, and Learning*, ITP, Beijing.
- October 2019 **Differentiable programming quantum physics and quantum circuits**, *4th International Symposium on Research and Education of Computational Science*, The Computational Science Alliance of the University of Tokyo, Japan.
- August 2019 **1. A hitchhiker's guide to machine learning, 2. Secrets of deep learning, 3. Generative models for physicists**, *Summer School on Machine Learning in Condensed Matter Physics*, DIPC San Sebastian, Spain.
- July 2021 **1. Scientific machine learning with and without data, 2. Generative models, 3. Differentiable programming**, *CRC 183 Summer School Machine Learning in Condensed Matter Physics*, Cologne, Germany.
- August 2021 **Two lessons from deep learning**, *Summer School: Machine Learning in Quantum Physics and Chemistry*, Warsaw, Poland.
- Dec 2022 **Generative AI for Science**, *127th CCF Advanced Disciplines Lectures: AI + Science*, Beijing, China.
- Spring 2023 **Machine learning for physicists**, *A crash course at IOP-CAS*, Beijing, China.
- Nov 2023 **Generative models for physicists**, *International conference on machine learning physics*, Kyoto, Japan.
- April 2025 **Autoregressive model: alphabets, actions, and atoms**, *The 13th Workshop on Quantum Many-Body Computation*, Hangzhou, China.

Students and Postdocs

- Postdoc **Jin-Guo Liu**, *HKUST-GZ*, Assistant Professor.
2017-2019
- Postdoc **Shuang Liang**, *IOPLY*, Manager.
2021-2023
- PhD **Shuo-Hui Li**, *HKUST*, Research Assistant Professor.
2015-2020
- PhD **Hong-Bin Ren**, *Baidu quantum*, Research scientist.
2016-2021 co-supervised with Prof. Xi Dai
- PhD **Wei Tang**, *Ghent University*, Postdoc.
2016-2021 co-supervised with Prof. Hong-Hao Tu and Prof. X. C. Xie
- PhD **Yueshui Zhang**, *LMU Munich*, Postdoc.
2017-2023
- PhD **Hao Xie**, *University of Zurich*, Postdoc.
2018-2023
- PhD **Xingyu Zhang**, *Ghent University*, Postdoc.
2019-2024
- PhD **Qi Yang**, *University of Amsterdam*, Postdoc.
2019-2024

PhD **Lu Zhao**.
2018-2024

Open Source Organizations

QuantumBFS **A group of quantum developers around Bao Fu Si.**
TensorBFS **Tensorize Everything!**
FermiFlow **Ab-initio study of fermions at finite temperature.**

Services

2020- **Chinese Physics Letter**, *Editorial Board Member*.
2021- **Science Bulletin**, *Executive Member of Editorial Board*.
2021- **Machine Learning: Science and Technology**, *Editorial Board Member*.
2022- **Journal of Machine Learning**, *Editorial Board Member*.
2025- **Physics**, *Editorial Board Member*.
2025- **AI for Science**, *Associate Editors*.

Grants

2018-2021 **Machine Learning and Many Body Physics**, *NSFC General Grant*, ¥680,000.
2021-2023 **Solving Many-electron Schrodinger Equations with Deep Learning**, *Huawei*, ¥140,000.
2023-2025 **Solving finite-temperature many-electron problem using deep generative model based variational free-energy method**, *NSFC Key Research Program*, ¥800,000.
2023-2027 **Machine Learning and Many Body Physics**, *NSFC Outstanding Young Scientists*, ¥4,000,000.
2025-2029 **Data- and Intelligence-Driven Quantum Materials Research**, *Beijing Natural Science Foundation Interdisciplinary Project*, ¥3,000,000.

Publications

- [1] **Lei Wang**, Xi Dai, Shu Chen, and X. C. Xie. *Magnetism of cold fermionic atoms on the p band of an optical lattice*. *Phys. Rev. A* **78**, 023603 (2008).
- [2] XiaoYu Deng, **Lei Wang**, Xi Dai, and Zhong Fang. *Local density approximation combined with Gutzwiller method for correlated electron systems: Formalism and applications*. *Phys. Rev. B* **79**, 075114 (2009).
- [3] Jia Ning Zhuang, **Lei Wang**, Zhong Fang, and Xi Dai. *Fast impurity solver based on Gutzwiller variational approach*. *Phys. Rev. B* **79**, 165114 (2009).
- [4] Hua Jiang, **Lei Wang**, Qing-feng Sun, and X. C. Xie. *Numerical study of the topological anderson insulator in HgTe/CdTe quantum wells*. *Phys. Rev. B* **80**, 165316 (2009).
- [5] **Lei Wang**, Hua Jiang, J. N. Zhuang, Xi Dai, and X. C. Xie. *Spin current through an ESR quantum dot: A real-time study*. *Phys. Rev. B* **81**, 075323 (2010).
- [6] Zi Cai, **Lei Wang**, X. C. Xie, and Yupeng Wang. *Interaction-induced anomalous transport behavior in one-dimensional optical lattices*. *Phys. Rev. A* **81**, 043602 (2010).
- [7] Jian-Qing Qi, **Lei Wang**, and Xi Dai. *Antiferromagnetism of repulsively interacting fermions in a harmonic trap*. *Chinese Physics Letters* **27**, 083102 (2010).

- [8] Zi Cai, **Lei Wang**, X. C. Xie, U. Schollwöck, X. R. Wang, M. Di Ventura, and Yupeng Wang. Quantum spinon oscillations in a finite one-dimensional transverse Ising model. *Phys. Rev. B* **83**, 155119 (2011).
- [9] **Lei Wang**, Xi Dai, and X. C. Xie. *Frequency domain winding number and interaction effect on topological insulators*. *Phys. Rev. B* **84**, 205116 (2011).
- [10] **Lei Wang**, Hua Jiang, Xi Dai, and X. C. Xie. *Pole expansion of self-energy and interaction effect for topological insulators*. *Phys. Rev. B* **85**, 235135 (2012).
- [11] **Lei Wang**, Xi Dai, and X. C. Xie. *Interaction-induced topological phase transition in the Bernevig-Hughes-Zhang model*. *Europhysics Letter* **98**, 57001 (2012).
- [12] Thomas Uehlinger, Daniel Greif, Gregor Jotzu, Leticia Tarruell, Tilman Esslinger, **Lei Wang** and Matthias Troyer. *Double transfer through Dirac points in a tunable honeycomb optical lattice*. *Eur. Phys. J. Special Topics*, **217**, 121 (2013). (Cover image)
- [13] Hsiang-Hsuan Hung, **Lei Wang**, Zheng-Cheng Gu and Gregory A. Fiete. *Topological phase transition in a generalized Kane-Mele-Hubbard model: A combined Quantum Monte Carlo and Green's function study*. *Phys. Rev. B* **87**, 121113(R) (2013).
- [14] **Lei Wang**, Alexey A. Soluyanov and Matthias Troyer. *Proposal for direct measurement of topological invariants in optical lattices*. *Phys. Rev. Lett* **110**, 166802 (2013).
- [15] Zi Cai, Hsiang-Hsuan Hung, **Lei Wang**, Dong Zheng and Congjun Wu. *Pomeranchuk cooling of the $SU(2N)$ ultra-cold fermions in optical lattices*. *Phys. Rev. Lett* **110**, 220401 (2013).
- [16] **Lei Wang**, Matthias Troyer and Xi Dai. *Topological charge pumping in a one-dimensional optical lattice*. *Phys. Rev. Lett* **111**, 026802 (2013).
- [17] Zi Cai, Hsiang-Hsuan Hung, **Lei Wang** and Congjun Wu. *Quantum magnetic properties of the $SU(2N)$ Hubbard model in the square lattice: a quantum Monte Carlo study*. *Phys. Rev. B* **88**, 125108 (2013).
- [18] **Lei Wang** and Matthias Troyer. *Seeing Hofstadter's Butterfly in Atomic Fermi Gases*. *Phys. Rev. A* **89**, 011603(R) (2014).
- [19] Jakub Imriška, Mauro Iazzi, **Lei Wang**, Emanuel Gull, Daniel Greif, Thomas Uehlinger, Gregor Jotzu, Leticia Tarruell, Tilman Esslinger and Matthias Troyer. *Thermodynamics and magnetic properties of the anisotropic 3D Hubbard model*, *Phys. Rev. Lett* **112**, 115301 (2014).
- [20] Hsiang-Hsuan Hung, Victor Chua, **Lei Wang** and Gregory A. Fiete. *Finite-size and interaction effects on topological phase transitions via numerically exact quantum Monte Carlo calculations*, *Phys. Rev. B* **89**, 235104 (2014).
- [21] **Lei Wang** and Matthias Troyer. *Renyi Entanglement Entropy of Interacting Fermions Calculated Using Continuous-Time Quantum Monte Carlo Method*, *Phys. Rev. Lett.* **113**, 110401 (2014).
- [22] **Lei Wang**, Philippe Corboz and Matthias Troyer. *Fermionic Quantum Critical Point of Spinless Fermions on a Honeycomb Lattice*, *New J. of Phys.*, **16**, 103008 (2014), selected by the Editors for IOPselect.
- [23] **Lei Wang**, Hsiang-Hsuan Hung and Matthias Troyer. *Topological Phase Transition in the Hofstadter-Hubbard Model*, *Phys. Rev. B* **90**, 205111 (2014).

- [24] **Lei Wang**, Mauro Iazzi, Philippe Corboz and Matthias Troyer. *Efficient Continuous-time Quantum Monte Carlo Method for the Ground State of Correlated Fermions*, Phys. Rev. B **91**, 235151 (2015), Editors' suggestion.
- [25] **Lei Wang**, Ye-Hua Liu, Jakub Imriška, Ping Nang Ma, Matthias Troyer. *Fidelity susceptibility made simple: A unified quantum Monte Carlo approach*, Phys. Rev. X **5**, 031007 (2015).
- [26] **Lei Wang**, Hiroshi Shinaoka, Matthias Troyer. *Fidelity Susceptibility Perspective on the Kondo Effect and Impurity Quantum Phase Transitions*, Phys. Rev. Lett. **115**, 236601 (2015).
- [27] Ye-Hua Liu and **Lei Wang**. *Quantum Monte Carlo study of mass-imbalanced Hubbard models*, Phys. Rev. B **92**, 235129 (2015), Editors' suggestion.
- [28] **Lei Wang**, Ye-Hua Liu, Mauro Iazzi, Matthias Troyer, Gergely Harcos. *Split orthogonal group: A guiding principle for sign-problem-free fermionic simulations*, Phys. Rev. Lett. **115**, 250601 (2015).
- [29] Shuta Nakajima, Takafumi Tomita, Shintaro Taie, Tomohiro Ichinose, Hideki Ozawa, **Lei Wang**, Matthias Troyer, Yoshiro Takahashi. *Topological Thouless Pumping of Ultracold Fermions*, Nature Physics **12**, 296 (2016).
- [30] **Lei Wang**, Ye-Hua Liu and Matthias Troyer. *Stochastic series expansion simulation of the t - V model*, Phys. Rev. B **93**, 155117 (2016).
- [31] Jakub Imriška, **Lei Wang**, Matthias Troyer. *First order topological phase transition of the Haldane–Hubbard model*, Phys. Rev. B **94**, 035109 (2016).
- [32] Ilya Zintchenko, **Lei Wang** and Matthias Troyer. *Ferromagnetism of the Repulsive Atomic Fermi Gas: three-body recombination and domain formation*, Eur. Phys. J. B **89**, 180 (2016)
- [33] **Lei Wang**, *Discovering Phase Transitions with Unsupervised Learning*, Phys. Rev. B **94**, 195105 (2016)
- [34] Li Huang, Yilin Wang, **Lei Wang**, Philipp Werner, *Detecting phase transitions and crossovers in Hubbard models using the fidelity susceptibility*, Phys. Rev. B **94**, 235110 (2016)
- [35] Li Huang, **Lei Wang**. *Accelerate Monte Carlo Simulations with Restricted Boltzmann Machines*, Phys. Rev. B **95**, 035105 (2017)
- [36] Li Huang, Yi-feng Yang, **Lei Wang**, *Recommender Engine for Continuous Time Quantum Monte Carlo Methods*, Phys. Rev. E **95**, 031301(R) (2017)
- [37] Jan Gukelberger, **Lei Wang**, and Lode Pollet, *Ising Antiferromagnet in the 2D Hubbard Model with Mismatched Fermi Surfaces*, Phys. Rev. B **95**, 205121 (2017)
- [38] Wei Tang, Lei Chen, Wei Li, X. C. Xie, Hong-Hao Tu, **Lei Wang**, *Universal Boundary Entropies in Conformal Field Theory: A Quantum Monte Carlo Study* Phys. Rev. B **96**, 115136 (2017), Editors' suggestion.
- [39] **Lei Wang**, *Exploring cluster Monte Carlo updates with Boltzmann machines* Phys. Rev. E **96**, 051301(R) (2017)
- [40] Lei Chen, Hao-Xin Wang, **Lei Wang**, Wei Li, *Conformal Thermal Tensor Network and Universal Entropy on Topological Manifolds*, Phys. Rev. B **96**, 174429 (2017)
- [41] Jing Chen, Song Cheng, Haidong Xie, **Lei Wang**, and Tao Xiang, *On the Equivalence of Restricted Boltzmann Machines and Tensor Network States*, Phys. Rev. B **97**, 085104 (2018), Editors' suggestion.

- [42] H.-M. Guo, **Lei Wang**, R. T. Scalettar, *Quantum phase transitions of multi-species Dirac fermions*, Phys. Rev. B **97**, 235152 (2018)
- [43] Zhao-Yu Han, Jun Wang, Heng Fan, **Lei Wang**, Pan Zhang, *Unsupervised Generative Modeling Using Matrix Product States*, Phys. Rev. X **8**, 031012 (2018)
- [44] Song Cheng, Jing Chen, **Lei Wang**, *Information Perspective to Probabilistic Modeling: Boltzmann Machines versus Born Machines*, Entropy **20**, 583 (2018)
- [45] Jin-Guo Liu, **Lei Wang**, *Differentiable Learning of Quantum Circuit Born Machine*, Phys. Rev. A **98**, 062324 (2018)
- [46] Shuo-Hui Li, **Lei Wang**, *Neural Network Renormalization Group*, Phys. Rev. Lett. **121**, 260601 (2018)
- [47] Wei Zhang, **Lei Wang**, and Ziqiang Wang, *Interpretable Machine Learning Study of Many-Body Localization Transition in Disordered Quantum Ising Spin Chains*, Phys. Rev. B **99**, 054208 (2019)
- [48] Dian Wu, **Lei Wang**, Pan Zhang, *Solving Statistical Mechanics using Variational Autoregressive Networks*, Phys. Rev. Lett. **122**, 080602 (2019), Editors' Suggestion
- [49] Wei Tang, X. C. Xie, **Lei Wang**, Hong-Hao Tu, *The Klein bottle entropy of the compactified boson conformal field theory*, Phys. Rev. B **99**, 115105 (2019)
- [50] Song Cheng, **Lei Wang**, Tao Xiang, Pan Zhang, *Tree Tensor Networks for Generative Modeling*, Phys. Rev. B **99**, 155131 (2019)
- [51] Jinfeng Zeng, Yufeng Wu, Jin-Guo Liu, **Lei Wang**, Jiangping Hu, *Learning and Inference on Generative Adversarial Quantum Circuits*, Phys. Rev. A **99**, 052306 (2019)
- [52] Tang-Shi Yao, Cen-Yao Tang, Meng Yang, Ke-Jia Zhu, Da-Yu Yan, Chang-Jiang Yi, Zi-Li Feng, He-Chang Lei, Cheng-He Li, Le Wang, **Lei Wang**, You-Guo Shi, Yu-Jie Sun, Hong Ding, *Machine Learning to Instruct Single Crystal Growth by Flux Method*, Chinese Physics Letters, **36**, 068101 (2019)
- [53] Hai-Jun Liao, Jin-Guo Liu, **Lei Wang**, Tao Xiang, *Differentiable Programming Tensor Networks*, Phys. Rev. X **9**, 031041 (2019)
- [54] Jin-Guo Liu, Yi-Hong Zhang, Yuan Wan, **Lei Wang**, *Variational Quantum Eigensolver with Fewer Qubits*, Phys. Rev. Research **1**, 023025 (2019)
- [55] Da Wang, **Lei Wang**, Congjun Wu, *Slater and Mott insulating states in the $SU(6)$ Hubbard model*, Phys. Rev. B **100**, 115155 (2019)
- [56] Wei Tang, X. C. Xie, **Lei Wang**, Hong-Hao Tu, *Quantized thermal Hall conductance from edge current calculations in the lattice model*, Phys. Rev. B **100**, 155112 (2019)
- [57] Romain Fournier, **Lei Wang**, Oleg V. Yazyev, QuanSheng Wu, *An Artificial Neural Network Approach to the Analytic Continuation Problem*, Phys. Rev. Lett. **124**, 056401 (2020)
- [58] Danqing Hu, Jian-Jun Dong, Li Huang, **Lei Wang**, Yi-feng Yang, *An effective classical correspondence of the Mott transition*, Phys. Rev. B **101**, 075111 (2020), Editors' Suggestion
- [59] Jun Wang, Zhao-Yu Han, Song-Bo Wang, Zeyang Li, Liang-Zhu Mu, Heng Fan, **Lei Wang**, *Efficient Quantum Tomography with Fidelity Estimation*, Phys. Rev. A **101**, 032321 (2020)
- [60] Shuo-Hui Li, Chen-Xiao Dong, Linfeng Zhang, **Lei Wang**, *Neural Canonical Transformation with Symplectic Flows*, Phys. Rev. X **10**, 021020 (2020)

- [61] Hao Xie, Jin-Guo Liu, **Lei Wang**, *Automatic differentiation of dominant eigensolver and its applications in quantum physics*, Phys. Rev. B **101**, 245139 (2020)
- [62] Ying-Hai Wu, **Lei Wang**, Hong-Hao Tu, *Tensor network representations of parton wave functions*, Phys. Rev. Lett. **124**, 246401 (2020)
- [63] Hong-Ye Hu, Shuo-Hui Li, **Lei Wang**, Yi-Zhuang You, *Machine Learning Holographic Mapping by Neural Network Renormalization Group*, Phys. Rev. Research **2**, 023369 (2020)
- [64] Bin-Bin Chen, Yuan Gao, Yi-Bin Guo, Yuzhi Liu, Hui-Hai Zhao, Hai-Jun Liao, **Lei Wang**, Tao Xiang, Wei Li, Z. Y. Xie, *Automatic Differentiation for Second Renormalization of Tensor Networks*, Phys. Rev. B **101**, 220409(R) (2020)
- [65] Xiu-Zhe Luo, Jin-Guo Liu, Pan Zhang, **Lei Wang**, *Yao.jl: Extensible, Efficient Framework for Quantum Algorithm Design*, Quantum **4**, 341 (2020)
- [66] Wei Tang, Hong-Hao Tu, **Lei Wang**, *Continuous matrix product operator approach to finite temperature quantum states*, Phys. Rev. Lett. **125**, 170604 (2020)
- [67] Jin-Guo Liu, Liang Mao, Pan Zhang, **Lei Wang**, *Solving Quantum Statistical Mechanics with Variational Autoregressive Networks and Quantum Circuits*, Machine Learning: Science and Technology **2**, 025011 (2021)
- [68] Jin-Guo Liu, **Lei Wang**, Pan Zhang, *Tropical Tensor Network for Ground States of Spin Glasses*, Phys. Rev. Lett. **126**, 090506 (2021)
- [69] Song Cheng, **Lei Wang**, Pan Zhang, *Supervised Learning with Projected Entangled Pair States*, Phys. Rev. B **103**, 125117 (2021)
- [70] Wei Tang, X. C. Xie, **Lei Wang**, Hong-Hao Tu, *Tensor network simulation of the (1+1)-dimensional $O(3)$ nonlinear σ -model with $\theta = \pi$ term*, Phys. Rev. D. **104**, 114513 (2021)
- [71] Hao Xie, Linfeng Zhang, **Lei Wang**, *Ab-initio study of interacting fermions at finite temperature with neural canonical transformation*, Journal of Machine Learning, **1**, 38 (2022)
- [72] Xiaotong Ni, Hui-Hai Zhao, **Lei Wang**, Feng Wu, Jianxin Chen, *Integrating Quantum Processor Device and Control Optimization in a Gradient-based Framework*, npj Quantum Inf **8**, 106 (2022)
- [73] Yueshui Zhang, **Lei Wang**, *Structure of continuous matrix product operator for transverse field Ising model: An analytic and numerical study*, Chinese Phys. B **31** 110205 (2022)
- [74] Xue-Yi Guo, Shang-Shu Li, Xiao Xiao, Zhong-Cheng Xiang, Zi-Yong Ge, He-Kang Li, Peng-Tao Song, Yi Peng, Kai Xu, Pan Zhang, **Lei Wang**, Dong-Ning Zheng, Heng Fan, *Thermal variational quantum simulation on a superconducting quantum processor*, Chinese Phys. B, **32** 010307 (2023)
- [75] Qi Yang, Xing-Yu Zhang, Hai-Jun Liao, Hong-Hao Tu, **Lei Wang**, *Projected d-wave superconducting state: a fermionic projected entangled pair state study*, Phys. Rev. B **107**, 125128 (2023)
- [76] Yueshui Zhang, Anton Hulsch, Hua-Chen Zhang, Wei Tang, **Lei Wang**, Hong-Hao Tu, *Universal scaling of Klein bottle entropy near conformal critical points*, Phys. Rev. Lett. **130**, 151602 (2023)
- [77] Hao Xie, Linfeng Zhang, **Lei Wang**, *m^* of two-dimensional electron gas: a neural canonical transformation study*, SciPost Phys. **14**, 154 (2023)

- [78] Stephan Humeniuk, Yuan Wan, **Lei Wang**, *Autoregressive neural Slater-Jastrow ansatz for variational Monte Carlo simulation*, SciPost Phys. **14**, 171 (2023)
- [79] Han Xu, Zhichao Zhou, Xin Wang, **Lei Wang**, Yu Wang, *Trion states and quantum criticality of attractive $SU(3)$ Dirac fermions*, Phys. Rev. Research **5**, 023180 (2023)
- [80] Xing-Yu Zhang, Shuang Liang, Hai-Jun Liao, Wei Li, **Lei Wang**, *Differentiable programming tensor networks for Kitaev magnets*, Phys. Rev. B **108**, 085103 (2023)
- [81] Hao Xie, Zi-Hang Li, Han Wang, Linfeng Zhang, **Lei Wang**, *A deep variational free energy approach to dense hydrogen*, Phys. Rev. Lett. **131**, 126501 (2023)
- [82] Zhanghao Zhouyin, Xiang Chen, Peng Zhang, Jun Wang, **Lei Wang**, *Automatic differentiable nonequilibrium Green's function formalism: An end-to-end differentiable quantum transport simulator*, Phys. Rev. B **108**, 195143 (2023)
- [83] Lu Zhao, **Lei Wang**, *Bounding free energy difference with flow matching*, Chinese Physics Letters, **40**, 120201 (2023)
- [84] Xihan Li, Xiang Chen, Rasul Tutunov, Haitham Bou-Ammar, **Lei Wang**, Jun Wang, *Online PCA in Converging Self-consistent Field Equations*, Thirty-seventh Conference on Neural Information Processing Systems (2023)
- [85] Xinyang Dong, Emanuel Gull, **Lei Wang**, *Equivariant neural network for Green's functions of molecules and materials*, Phys. Rev. B **109**, 075112 (2024)
- [86] Xing-Yu Zhang, Runze Chi, Yang Liu, **Lei Wang**, *Two-dimensional excitation information by a matrix product state method on infinite helices*, Phys. Rev. B **109**, 075129 (2024)
- [87] Qi Zhang, Rui-Si Wang, **Lei Wang**, *Neural canonical transformations for vibrational spectra of molecules*, J. Chem. Phys. **161**, 024103 (2024)
- [88] Dian Wu et al, *Variational Benchmarks for Quantum Many-Body Problems*, Science, **386**, 296 (2024)
- [89] Bi-Yang Tan, Yueshui Zhang, Hua-Chen Zhang, Wei Tang, **Lei Wang**, Hong-Hao Tu, Ying-Hai Wu, *Extracting the Luttinger parameter from a single wave function*, Phys. Rev. Lett. **134**, 076501 (2025)
- [90] Yuwei Ma, Weiting Wang, Xianghao Mu, Weizhou Cai, Ziyue Hua, Xiaoxuan Pan, Dong-Ling Deng, Rebing Wu, Chang-Ling Zou, **Lei Wang**, Luyan Sun, *Experimental Implementation of a Qubit-Efficient Variational Quantum Eigensolver with Analog Error Mitigation on a Superconducting Quantum Processor*, Science China, Physics, Mechanics and Astronomy, **68**, 270311 (2025)
- [91] Qi Zhang, Xiaoyang Wang, Rong Shi, Xinguo Ren, Han Wang, **Lei Wang**, *Neural Canonical Transformations for Quantum Anharmonic Solids of Lithium*, Phys. Rev. Lett. **134**, 246101 (2025)
- [92] Xinyang Dong, Hao Xie, Yixiao Chen, Wenshuo Liang, Linfeng Zhang, **Lei Wang**, Han Wang, *Discovering dense hydrogen solid at 1200K with deep variational free energy approach*, Phys. Rev. B **111**, 214118 (2025)
- [93] Xing-Yu Zhang, Yu-Qing Wang, Angrui Du, Han Wang, **Lei Wang**, Jinguo Liu, *Dynamic Hologram Generation with Automatic Differentiation*, Phys. Rev. Applied **24**, 024011 (2025)
- [94] Zhendong Cao, Xiaoshan Luo, Jian Lv, **Lei Wang**, *Space Group Informed Transformer for Crystalline Materials Generation*, Science Bulletin **70**, 3522 (2025)

- [95] Xiaoshan Luo, Zhenyu Wang, Jian Lv, **Lei Wang**, Yanchao Wang, Yanming Ma, *CrystalFlow: A Flow-Based Generative Model for Crystalline Materials*, Nature Communications **16**, 9267 (2025)
- [96] Qi Zhang, **Lei Wang**, *Quantum Anharmonic Effects in Hydrogen-Bond Symmetrization of High-Pressure Ice*, Phys. Rev. B **112**, 174106 (2025)
- [97] Yantao Wu, Zhehao Dai, Sajant Anand, Sheng-Hsuan Lin, Qi Yang, **Lei Wang**, Frank Pollmann, Michael P. Zaletel, *Alternating and Gaussian fermionic Isometric Tensor Network States*, PRX Quantum **6**, 040324 (2025)
- [98] Caiyuan Ye, Yuzhi Wang, Xintian Xie, Tiannian Zhu, Jiaxuan Liu, Yuqing He, Lili Zhang, Junwei Zhang, Zhong Fang, **Lei Wang**, Zhipan Liu, Hongming Weng, Quansheng Wu, *Materials discovery acceleration by using condition generative methodology*, arXiv:2505.00076, npj Computational Materials (2025)
- [99] Zhendong Cao, **Lei Wang**, *Reinforcement Fine-Tuning for Materials Design*, Phys. Rev. B **113**, 024106 (2026)
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