Inverse Problems Symposium 2025

Name: Alexander Benedix Robles
Organization: Center for Advanced Systems Understanding

Abstract Title: PyLIT: Reformulation and implementation of the analytic continuation problem using kernel representation methods.

Authors: Alexander Benedix Robles, Phil-Alexander Hofmann, Thomas Chuna, Tobias Dornheim, Michael Hecht

Alexander Benedix Robles,1, 2, 3, Phil-Alexander Hofmann,1, 2, †
Thomas Chuna,1, 2, ‡ Tobias Dornheim,1, 2, § and Michael Hecht1, 2, ¶

1Center for Advanced Systems Understanding (CASUS), D-02826 G¨orlitz, Germany
2Helmholtz-Zentrum Dresden-Rossendorf (HZDR), D-01328 Dresden, Germany
3Technische Universit¨at Dresden, D-01062 Dresden, Germany

Abstract:

Path integral Monte Carlo (PIMC) simulations are a cornerstone method for studying quantum many-body systems, such as warm dense matter [1, 2] and ultracold atoms [3, 4]. The exponentially ill-posed inverse Laplace transform [5, 6] impedes extracting dynamical observables such as the dynamic structure factor S(q, E)—a key property e.g. in x-ray and neutron scattering experiments—from PIMC data for the imaginary-time correlation function F (q, τ). Despite numerous attempts [3, 4, 7–21], no universally accepted approach has been identified to solve this problem and many methods remain unsatisfactory.

To address the limitations of the commonly posed optimization problem, we propose alternative formulations that improve the conditioning and intro-duce a more robust and physically meaningful regression approach, thereby enhancing the reliability of the solution.Specifically, we express the solution as a linear combination of kernels with automatically enforced detailed balance (a weighted symmetry property). In combination with prior knowledge of the shape of S(q, E), we implement regularization methods typical to this field (L1, and MaxEnt) and implement a hitherto unexplored regularizer according to Wasserstein distance.

As a key outcome, we developed the open-source Python library PyLIT (Python Laplace Inverse Transform), which provides an accessible tool for the determination of the relevant meta-parameters of the kernel basis and for the inversion of the two-sided Laplace transform to obtain reliable results for S(q, E) from F (q, τ).We have gained several insights from the new formula-tions. First, the results highlight the importance of hyperparameter selection, which is essential for achieving strong performance and may also offer a means to improve classical formulations. Second, a way to combine the strengths of regularized and stochastic optimization was identified: by applying stochastic optimization to the basis, the conditioning of regularized problems—such as in analytic continuation—can be improved.

ACKNOWLEDGMENTS

ABR, PAH and TC contributed equally to this work. TC acknowledges Tom Gawne for insightful discussions on HPC and node-to-node communication. This work was partially supported by the Center for Advanced Systems Understanding (CASUS), financed by Germany's Federal Ministry of Education and Research (BMBF) and the Saxon state government out of the State budget approved by the Saxon State Parliament. This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2022 research and innovation programme (Grant agreement No. 101076233, "PREXTREME"). Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or the European Research Council Executive Agency. Neither the European Union nor the granting authority can be held responsible for them. This work has received funding from the European Union's Just Transition Fund (JTF) within the project *Röntgenlaser-Optimierung der Laserfusion* (ROLF), contract number 5086999001, co-financed by the Saxon state government out of the State budget approved by the Saxon State Parliament. Computations were performed on a Bull Cluster at the Center for Information Services and High-Performance Computing (ZIH) at Technische Universität Dresden, at the Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen (HLRN) under grant mvp00024, and on the HoreKa supercomputer funded by the Ministry of Science, Research and the Arts Baden-Württemberg and by the Federal Ministry of Education and Research.

---

[1] S. H. Glenzer and R. Redmer, "X-ray thomson scattering in high energy density plasmas," Rev. Mod. Phys **81**, 1625 (2009).

[2] Tobias Dornheim, Zhandos A. Moldabekov, Kushal Ramakrishna, Panagiotis Tolias, Andrew D. Baczewski, Dominik Kraus, Thomas R. Preston, David A. Chapman, Maximilian P. Böhme, Tilo Döppner, Frank Graziani, Michael Bonitz, Attila Cangi, and Jan Vorberger, "Electronic density response of warm dense matter," Physics of Plasmas **30**, 032705 (2023).

[3] G. Ferré and J. Boronat, "Dynamic structure factor of liquid ^{4}He across the normal-superfluid transition," Phys. Rev. B **93**, 104510 (2016).

[4] A. Filinov and M. Bonitz, "Collective and single-particle excitations in two-dimensional dipolar bose gases," Phys. Rev. A **86**, 043628 (2012).

[5] Charles L Epstein and John Schotland, "The bad truth about laplace's transform," SIAM review **50**, 504–520 (2008).

[6] Andrei A Istratov and Oleg F Vyvenko, "Exponential analysis in physical phenomena," Review of Scientific Instruments **70**, 1233–1257 (1999).

[7] Mark Jarrell and J.E. Gubernatis, "Bayesian inference and the analytic continuation of imaginary-time quantum monte carlo data," Physics Reports **269**, 133–195 (1996).

[8] Youssef Kora and Massimo Boninsegni, "Dynamic structure factor of superfluid ^{4}He from quantum monte carlo: Maximum entropy revisited," Phys. Rev. B **98**, 134509 (2018).

[9] R. N. Silver, D. S. Sivia, and J. E. Gubernatis, "Maximum-entropy method for analytic continuation of quantum monte carlo data," Phys. Rev. B **41**, 2380–2389 (1990).

[10] Thomas Chuna, Nicholas Barnfield, Tobias Dornheim, Michael P Friedlander, and Tim Hoheisel, "Dual formulation of the maximum entropy method applied to analytic continuation of quantum monte carlo data," arXiv preprint arXiv:2501.01869 (2025).

[11] Thomas Chuna, Nicholas Barnfield, Jan Vorberger, Michael P Friedlander, Tim Hoheisel, and Tobias Dornheim, "Estimates of the dynamic structure factor for the finite temperature electron liquid via analytic continuation of path integral monte carlo data," arXiv preprint arXiv:2503.20433 (2025).

[12] Stephen F Gull, "Developments in maximum entropy data analysis," in *Maximum Entropy and Bayesian Methods: Cambridge, England, 1988* (Springer, 1989) pp. 53–71.

[13] Josef Kaufmann and Karsten Held, "ana_cont: Python package for analytic continuation," Computer Physics Communications **282**, 108519 (2023).

[14] Yannis Burnier and Alexander Rothkopf, "Bayesian approach to spectral function reconstruction¡? format?¿ for euclidean quantum field theories," Physical review letters **111**, 182003 (2013).

[15] Junya Otsuki, Masayuki Ohzeki, Hiroshi Shinaoka, and Kazuyoshi Yoshimi, "Sparse modeling approach to analytical continuation of imaginary-time quantum monte carlo data," Phys. Rev. E **95**, 061302 (2017).

[16] Junya Otsuki, Masayuki Ohzeki, Hiroshi Shinaoka, and Kazuyoshi Yoshimi, "Sparse modeling in quantum many-body problems," Journal of the Physical Society of Japan **89**, 012001 (2020), https://doi.org/10.7566/JPSJ.89.012001.

[17] A. S. Mishchenko, N. V. Prokof'ev, A. Sakamoto, and B. V. Svistunov, "Diagrammatic quantum monte carlo study of the fröhlich polaron," Phys. Rev. B **62**, 6317–6336 (2000).

[18] E. Vitali, M. Rossi, L. Reatto, and D. E. Galli, "Ab initio low-energy dynamics of superfluid and solid ^{4}He," Phys. Rev. B **82**, 174510 (2010).

[19] A. Filinov, "Correlation effects and collective excitations in bosonic bilayers: Role of quantum statistics, superfluidity, and the dimerization transition," Phys. Rev. A **94**, 013603 (2016).

[20] Hai-Tao Shu, Heng-Tong Ding, Olaf Kaczmarek, Swagato Mukherjee, and Hiroshi Ohno, "A stochastic approach to the reconstruction of spectral functions in lattice qcd," arXiv preprint arXiv:1510.02901 (2015).

[21] Tobias Dornheim, Zhandos A. Moldabekov, Jan Vorberger, and Burkhard Militzer, "Path integral monte carlo approach to the structural properties and collective excitations of liquid ^{3}he without fixed nodes," Scientific Reports **12**, 708 (2022).