

List of publications

Christian Schilling 



1 Publications and recent preprints

56. ***A toolbox of spin-adapted generalized Pauli constraints*** (2025)
Julia Liebert, Yannick Lemke, Murat Altunbulak, Tomasz Maciazek, Christian Ochsenfeld, [Christian Schilling](#)
Phys. Rev. Research 7, 023247 (2025)
55. ***Refining ensemble N -representability of one-body density matrices from partial information*** (2025)
Julia Liebert, Anna O. Schouten, Irma Avdic, [Christian Schilling](#), David A. Mazziotti
arXiv:2506.09960
54. ***Spin adaptation of the cumulant expansions of reduced density matrices*** (2025)
Julia Liebert, [Christian Schilling](#), David A. Mazziotti
arXiv:2505.16989, to appear in J. Chem. Phys.
53. ***From Entanglement to Bonds: Chemical Bonding Concepts from Quantum Information Theory*** (2025)
Lexin Ding, Eduard Matito, [Christian Schilling](#)
arXiv:2501.15699, sent out for review at Nat. Commun.
52. ***How to Incorporate Symmetries in Functional Theories*** (2025)
Julia Liebert, Tomasz Maciazek, [Christian Schilling](#)
submitted <https://www.dropbox.com/scl/fi/n9z5w5o7aspk5mpfwijys/RDMFTspin-JCTC-v8.pdf?rlkey=rxfy8d916h3qro6gnfqmn97m&dl=0>
51. ***A Spin-Faithful and Irreducible One-Matrix Functional Theory*** (2025)
Julia Liebert, Tomasz Maciazek, [Christian Schilling](#)
submitted <https://www.dropbox.com/scl/fi/kv5mgumlax1wh2p3htpr3/RDMFTspin-PRL-v8.pdf?rlkey=6pwz6shjnh7c04z2uth6kypwl&dl=0>

50. ***Solving one-body ensemble N -representability problems with spin*** (2024)
Julia Liebert, Federico Castillo, Jean-Philippe Labbé, Tomasz Maciazek, [Christian Schilling](#)
arXiv:2412.01805
49. ***Unveiling Intrinsic Many-Body Complexity by Compressing Single-Body Triviality*** (2024)
Ke Liao, Lexin Ding, [Christian Schilling](#)
J. Phys. Chem. Lett. 15, 6782
48. ***What can Quantum Information Theory Offer to Quantum Chemistry?*** (2024)
Damiano Aliverti-Piuri, Kaustav Chatterjee, Lexin Ding, Ke Liao, Julia Liebert, [Christian Schilling](#)
Faraday Discuss. 254, 76
47. ***Functional theory for quantum phase transitions*** (2024)
Martin Uttendorfer, Julia Liebert, [Christian Schilling](#)
submitted, <https://www.dropbox.com/scl/fi/gaqlpevzbk77shpzsr5q/FT-QPT-v5.pdf?rlkey=nz8lgkrkdim8iz21v0mzmfu55&dl=0>
46. ***Ground and Excited States from Ensemble Variational Principles*** (2024)
Lexin Ding, Cheng-Lin Hong, [Christian Schilling](#)
Quantum 8, 1525
45. ***Quantum Information-Assisted Complete Active Space Optimization (QICAS)*** (2023)
Lexin Ding, Stefan Knecht, [Christian Schilling](#)
J. Phys. Chem. Lett. 14, 49, 11022
44. ***Refining the weighted subspace-search variational quantum eigensolver: compression of ansätze into a single pure state and optimization of weights*** (2023)
Cheng-Lin Hong, Luis Colmenarez, Lexin Ding, Carlos L. Benavides-Riveros, [Christian Schilling](#)
arXiv:2306.11844, to appear in Phys. Rev. Research
43. ***Physical Entanglement Between Localized Orbitals*** (2023)
Lexin Ding, Gesa Dünneweber, [Christian Schilling](#)
Quantum Sci. Technol. 9, 015005
42. ***An effective solution to convex 1-body N -representability*** (2023)
Federico Castillo, Jean-Philippe Labbé, Julia Liebert, Arnau Padrol, Eva Philippe, [Christian Schilling](#)
Ann. Henri Poincaré 24, 2241

41. ***Refining and relating fundamentals of functional theory*** (2023)
Julia Liebert, Adam Y. Chaou, [Christian Schilling](#)
J. Chem. Phys. 158, 214108
40. ***Deriving density-matrix functionals for excited states*** (2023)
Julia Liebert, [Christian Schilling](#)
SciPost Phys. 14, 120
39. ***An exact one-particle theory of bosonic excitations: From a generalized Hohenberg-Kohn theorem to convexified N-representability*** (2023)
Julia Liebert, [Christian Schilling](#)
New J. Phys. 25, 013009
38. ***1-matrix functional for long-range interaction energy of two hydrogen atoms*** (2023)
Jerzy Cioslowski, [Christian Schilling](#), Rolf Schilling
J. Chem. Phys. 158, 084106
as Editor's pick
37. ***Quantum correlations in molecules: from quantum resourcing to chemical bonding*** (2023)
Lexin Ding, Stefan Knecht, Zoltán Zimborás, [Christian Schilling](#)
Quantum Sci. Technol. 8, 015015
36. ***Quantifying Electron Entanglement Faithfully*** (2022)
Lexin Ding, Zoltán Zimborás, [Christian Schilling](#)
arXiv:2207.03377, sent out for review at Nat. Commun.
35. ***Excitations of Quantum Many-Body Systems via Purified Ensembles: A Unitary-Coupled-Cluster-based Approach*** (2022)
Carlos L. Benavides-Riveros, Lipeng Chen, [Christian Schilling](#), Sebastián Mantilla, Stefano Pittalis
Phys. Rev. Lett. 129, 066401
with Editors' Suggestion
34. ***Foundation of one-particle reduced density matrix functional theory for excited states*** (2021)
Julia Liebert, Federico Castillo, Jean-Philippe Labbé, [Christian Schilling](#)
J. Chem. Theory Comput. 18, 1, 124

33. ***Ensemble reduced density matrix functional theory for excited states and hierarchical generalization of Pauli's exclusion principle*** (2021)
[Christian Schilling](#), Stefano Pittalis
Phys. Rev. Lett. 127, 023001
32. ***Fermionic systems for quantum information people*** (2021)
Szilárd Szalay, Zoltán Zimborás, Mihály Máté, Gergely Barcza, [Christian Schilling](#), Örs Legeza
J. Phys. A: Math. Theor. 54, 393001
31. ***Functional Theory for Bose-Einstein Condensates*** (2021)
Julia Liebert, [Christian Schilling](#)
Phys. Rev. Research 3, 013282
30. ***How creating one additional well can generate Bose-Einstein condensation*** (2021)
Mihály Máté, Örs Legeza, Rolf Schilling, Mason Yousif, [Christian Schilling](#)
Commun. Phys. 4, 29
29. ***Concept of orbital entanglement and correlation in quantum chemistry*** (2021)
Lexin Ding, Sam Mardazad, Sreetama Das, Szilárd Szalay, Ulrich Schollwöck, Zoltán Zimborás, [Christian Schilling](#)
J. Chem. Theory Comput. 17, 1, 79
28. ***Reduced Density Matrix Functional Theory for Bosons*** (2020)
Carlos L. Benavides-Riveros, Jakob Wolff, Miguel A. L. Marques, [Christian Schilling](#)
Phys. Rev. Lett. 124, 180603
27. ***Correlation paradox of the dissociation limit: A quantum information perspective*** (2020)
Lexin Ding, [Christian Schilling](#)
J. Chem. Theory Comput. 16, 4159
26. ***Implications of pinned occupation numbers for natural orbital expansions. II: Rigorous derivation and extension to non-fermionic systems*** (2020)
Tomasz Maciazek, Adam Sawicki, David Gross, Alexandre Lopes, [Christian Schilling](#)
New J. Phys. 22, 023002
25. ***Implications of pinned occupation numbers for natural orbital expansions. I: Generalizing the concept of active spaces*** (2020)
[Christian Schilling](#), Carlos L. Benavides-Riveros, Alexandre Lopes, Tomasz Maciazek, Adam Sawicki
New J. Phys. 22, 023001

24. ***Diverging exchange force and the form of density matrix functionals*** (2019)
[Christian Schilling](#), Rolf Schilling
Phys. Rev. Lett. 122, 013001
23. ***Communication: Relating the pure and ensemble density matrix functional*** (2018)
[Christian Schilling](#)
J. Chem. Phys. 149, 231102
22. ***Role of the pair potential for the saturation of generalized Pauli constraints*** (2018)
Örs Legeza, [Christian Schilling](#)
Phys. Rev. A 97, 052105
21. ***Generalized Pauli constraints in small atoms*** (2018)
[Christian Schilling](#), Murat Altunbulak, Stefan Knecht, Alexandre Lopes, James D. Whitfield, Matthias Christandl, David Gross, Markus Reiher
Phys. Rev. A 97, 052503
20. ***Reconstructing quantum states from single-party information*** (2017)
[Christian Schilling](#), Carlos Benavides-Riveros, Peter Vrana
Phys. Rev. A 96, 052312
19. ***Universal upper bounds on the Bose-Einstein condensate and the Hubbard star*** (2017)
Felix Tennie, Vlatko Vedral, [Christian Schilling](#)
Phys. Rev. B 96, 064502
18. ***Relating correlation measures: the importance of the energy gap*** (2017)
Carlos Benavides-Riveros, [Christian Schilling](#), Nektarios Lathiotakis, Miguel Marques
Phys. Rev. A 95, 032507
17. ***Influence of the fermionic exchange symmetry beyond Pauli's exclusion principle*** (2016)
Felix Tennie, Vlatko Vedral, [Christian Schilling](#)
Phys. Rev. A 95, 022336
16. ***Pinning of Fermionic Occupation Numbers: Higher Spatial Dimensions and Spin*** (2016)
Felix Tennie, Vlatko Vedral, [Christian Schilling](#)
Phys. Rev. A 94, 012120
15. ***Pinning of Fermionic Occupation Numbers: General Concepts and One Spatial Dimension*** (2016)
Felix Tennie, Daniel Ebler, Vlatko Vedral, [Christian Schilling](#)
Phys. Rev. A 93, 042126

14. ***Natural Extension of Hartree-Fock through extremal 1-fermion information: Overview and application to the lithium atom*** (2016)
 Carlos Benavides-Riveros, [Christian Schilling](#)
 Z. Phys. Chem. 230, 703-717
13. ***Number-parity effect for confined fermions in one dimension*** (2016)
[Christian Schilling](#), Rolf Schilling
 Phys. Rev. A 93, 021601, Rapid Communication
12. ***Hubbard model: Pinning of occupation numbers and role of symmetries*** (2015)
[Christian Schilling](#)
 Phys. Rev. B 92, 155149
11. ***Quasipinning and its relevance for N -Fermion quantum states*** (2015)
[Christian Schilling](#)
 Phys. Rev. A 91, 022105
10. ***Duality of reduced density matrices and their eigenvalues*** (2014)
[Christian Schilling](#), Rolf Schilling
 J. Phys. A 47, 415305
9. ***Natural Orbitals and Occupation Numbers for Harmonium: Fermions versus Bosons*** (2013)
[Christian Schilling](#)
 Phys. Rev. A 88, 042105
8. ***Pinning of Fermionic Occupation Numbers*** (2013)
[Christian Schilling](#), David Gross, and Matthias Christandl
 Phys. Rev. Lett. 110, 040404
 with Editors' Suggestion and Viewpoint in Physics

2 Proceedings and other contributions

7. ***Stochastic and low-scaling techniques: general discussion*** (2024)
 Ali Alavi, ..., [Christian Schilling](#), ..., Martijn A Zwijnenburg (46 contributors)
 Faraday Discuss. 451, 191
6. ***Novel perturbative and variational methods for stronger correlations: general discussion*** (2024)

Vibin Abraham, . . . , [Christian Schilling](#), . . . , Dominika Zgid (30 contributors)
Faraday Discuss. 254, 191

5. ***Comment on "Self-Consistent-Field Method for Correlated Many-Electron Systems with an Entropic Cumulant Energy"*** (2022)

Lexin Ding, Julia Liebert, [Christian Schilling](#)
arXiv:2202.05532

4. ***Introduction to Fermionic Entanglement and Correlation*** (2021)

[Christian Schilling](#)

Proceedings of the Autumn school "Simulating Correlations with Computers", Vol. 11, edited by E.Pavarini and E.Koch, Jülich, Germany

3. **The Quantum Marginal Problem** (2014)

[Christian Schilling](#)

Mathematical Results in Quantum Mechanics 10, 165, World Scientific

3 Software codes and packages

2. **MEAO: A package for electronic structure analysis based on maximally entangled atomic orbitals** (2025)

Lexin Ding, Eduard Matito, [Christian Schilling](#)

available upon request, soon to be released on <https://github.com/schilling-group>

1. **QIO: Quantum information-assisted orbital optimization package** (2024)

Lexin Ding, Ke Liao, [Christian Schilling](#)

<https://github.com/schilling-group>