

List of publications and recent preprints

Christian Schilling 



46. ***What can Quantum Information Theory Offer to Quantum Chemistry?*** (2024)
Damiano Aliverti-Piuri, Kaustav Chatterjee, Lexin Ding, Ke Liao, Julia Liebert, [Christian Schilling](#)
arXiv:2403.08045
45. ***Unveiling Intrinsic Many-Body Complexity by Compressing Single-Body Triviality*** (2024)
Ke Liao, Lexin Ding, [Christian Schilling](#)
arXiv:2402.16841
44. ***Ground and Excited States from Ensemble Variational Principles*** (2024)
Lexin Ding, Cheng-Lin Hong, [Christian Schilling](#)
arXiv:2401.12104
43. ***Quantum Information-Assisted Complete Active Space Optimization (QICAS)*** (2023)
Lexin Ding, Stefan Knecht, [Christian Schilling](#)
J. Phys. Chem. Lett. 14, 49, 11022
42. ***Functional theory for quantum phase transitions*** (2023)
Martin Uttendorfer, Julia Liebert, [Christian Schilling](#)
forthcoming
41. ***A Spin-Faithful and Irreducible One-Matrix Functional Theory*** (2023)
Julia Liebert, T.Maciazek, [Christian Schilling](#)
forthcoming
40. ***Quantum Parallelized Variational Quantum Eigensolvers for Excited States*** (2023)
Cheng-Lin Hong, Luis Colmenarez, Lexin Ding, Carlos L. Benavides-Riveros, [Christian Schilling](#)
arXiv:2306.11844
39. ***Physical Entanglement Between Localized Orbitals*** (2023)
Lexin Ding, Gesa D nnweber, [Christian Schilling](#)
Quantum Sci. Technol. 9, 015005

38. ***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 Poincare 24, 2241
37. ***Refining and relating fundamentals of functional theory*** (2023)
Julia Liebert, Adam Y. Chaou, [Christian Schilling](#)
J. Chem. Phys. 158, 214108
36. ***Deriving density-matrix functionals for excited states*** (2023)
Julia Liebert, [Christian Schilling](#)
SciPost Phys. 14, 120
35. ***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
34. ***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
33. ***Quantum correlations in molecules: from quantum resourcing to chemical bonding*** (2023)
Lexin Ding, Stefan Knecht, Zoltán Zimborás, [Christian Schilling](#)
Quantum Sci. Technol. 8, 015015
32. ***Quantifying Electron Entanglement Faithfully*** (2022)
Lexin Ding, Zoltán Zimborás, [Christian Schilling](#)
arXiv:2207.03377
31. ***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

30. ***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
29. ***Foundation of one-particle reduced density matrix functional theory for excited states*** (2021)
Julia Liebert, Frederico Castillo, Jean-Philippe Labbé, [Christian Schilling](#)
J. Chem. Theory Comput. 18, 1, 124
28. ***Introduction to Fermionic Entanglement and Correlation*** (2021)
[Christian Schilling](#)
to appear in the Proceedings of the Autumn school "Simulating Correlations with Computers", Vol. 11, edited by E.Pavarini and E.Koch, Jülich, Germany
27. ***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
26. ***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
25. ***Functional Theory for Bose-Einstein Condensates*** (2021)
Julia Liebert, [Christian Schilling](#)
Phys. Rev. Research 3, 013282
24. ***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
23. ***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
22. ***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

21. ***Correlation paradox of the dissociation limit: A quantum information perspective*** (2020)
Lexin Ding, [Christian Schilling](#)
J. Chem. Theory Comput. 16, 4159
20. ***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
19. ***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
18. ***Diverging exchange force and the form of density matrix functionals*** (2019)
[Christian Schilling](#), Rolf Schilling
Phys. Rev. Lett. 122, 013001
17. ***Communication: Relating the pure and ensemble density matrix functional*** (2018)
[Christian Schilling](#)
J. Chem. Phys. 149, 231102
16. ***Role of the pair potential for the saturation of generalized Pauli constraints*** (2018)
Örs Legeza, [Christian Schilling](#)
Phys. Rev. A 97, 052105
15. ***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
14. ***Reconstructing quantum states from single-party information*** (2017)
[Christian Schilling](#), Carlos Benavides-Riveros, Peter Vrana
Phys. Rev. A 96, 052312
13. ***Universal upper bounds on the Bose-Einstein condensate and the Hubbard star*** (2017)
Felix Tennie, Vlatko Vedral, [Christian Schilling](#)
Phys. Rev. B 96, 064502

12. ***Relating correlation measures: the importance of the energy gap*** (2017)
Carlos Benavides-Riveros, [Christian Schilling](#), Nektarios Lathiotakis, Miguel Marques
Phys. Rev. A 95, 032507
11. ***Influence of the fermionic exchange symmetry beyond Pauli's exclusion principle*** (2016)
Felix Tennie, Vlatko Vedral, [Christian Schilling](#)
Phys. Rev. A 95, 022336
10. ***Pinning of Fermionic Occupation Numbers: Higher Spatial Dimensions and Spin*** (2016)
Felix Tennie, Vlatko Vedral, [Christian Schilling](#)
Phys. Rev. A 94, 012120
9. ***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
8. ***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
7. ***Number-parity effect for confined fermions in one dimension*** (2016)
[Christian Schilling](#), Rolf Schilling
Phys. Rev. A 93, 021601, Rapid Communication
6. ***Hubbard model: Pinning of occupation numbers and role of symmetries*** (2015)
[Christian Schilling](#)
Phys. Rev. B 92, 155149
5. ***Quasipinning and its relevance for N -Fermion quantum states*** (2015)
[Christian Schilling](#)
Phys. Rev. A 91, 022105
4. ***Duality of reduced density matrices and their eigenvalues*** (2014)
[Christian Schilling](#), Rolf Schilling
J. Phys. A 47, 415305
3. **The Quantum Marginal Problem** (2014)
[Christian Schilling](#)
Mathematical Results in Quantum Mechanics 10, World Scientific

2. *Natural Orbitals and Occupation Numbers for Harmonium: Fermions versus Bosons* (2013)
[Christian Schilling](#)
Phys. Rev. A 88, 042105
1. *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