

# List of publications and recent preprints

- **Quantum correlations in molecules: A quantum information toolbox for chemists** (2022)  
Lexin Ding, Stefan Knecht, Zoltán Zimborás, Christian Schilling  
arXiv:2205.15881
- **Functional Theory for Excitations in Boson Systems** (2022)  
Julia Liebert, Christian Schilling  
arXiv:2204.12715
- **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
- **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  
arXiv:2201.10974
- **Foundation of one-particle reduced density matrix functional theory for excited states** (2021)  
Julia Liebert, Frederico Castillo, Jean-Philippe Labbé, Christian Schilling  
arXiv:2106.03918
- **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
- **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
- **Entanglement between orbitals in many-electron systems** (2021)  
Lexin Ding, Zoltán Zimborás, Christian Schilling  
Jul 2021, forthcoming

- **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
- **Functional Theory for Bose-Einstein Condensates** (2021)  
Julia Liebert, Christian Schilling  
Phys. Rev. Research 3, 013282
- **Realizing Bose-Einstein condensation in a Mexican-hat-like potential** (2021)  
Mihály Máté, Örs Legeza, Rolf Schilling, Mason Yousif, Christian Schilling  
Commun. Phys. 4, 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
- **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
- **Correlation paradox of the dissociation limit: A quantum information perspective** (2020)  
Lexin Ding, Christian Schilling  
J. Chem. Theory Comput. 16, 4159
- **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
- **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
- **Diverging exchange force and the form of density matrix functionals** (2019)  
Christian Schilling, Rolf Schilling  
Phys. Rev. Lett. 122, 013001
- **Communication: Relating the pure and ensemble density matrix functional** (2018)  
Christian Schilling  
J. Chem. Phys. 149, 231102

- **Role of the pair potential for the saturation of generalized Pauli constraints** (2018)  
Örs Legeza, Christian Schilling  
Phys. Rev. A 97, 052105
- **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
- **Reconstructing quantum states from single-party information** (2017)  
Christian Schilling, Carlos Benavides-Riveros, Peter Vrana  
Phys. Rev. A 96, 052312
- **Universal upper bounds on the Bose-Einstein condensate and the Hubbard star** (2017)  
Felix Tennie, Vlatko Vedral, Christian Schilling  
Phys. Rev. B 96, 064502
- **Relating correlation measures: the importance of the energy gap** (2017)  
Carlos Benavides-Riveros, Christian Schilling, Nektarios Lathiotakis, Miguel Marques  
Phys. Rev. A 95, 032507
- **Influence of the fermionic exchange symmetry beyond Pauli's exclusion principle** (2016)  
Felix Tennie, Vlatko Vedral, Christian Schilling  
Phys. Rev. A 95, 022336
- **Pinning of Fermionic Occupation Numbers: Higher Spatial Dimensions and Spin** (2016)  
Felix Tennie, Vlatko Vedral, Christian Schilling  
Phys. Rev. A 94, 012120
- **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
- **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
- **Number-parity effect for confined fermions in one dimension** (2016)  
Christian Schilling, Rolf Schilling  
Phys. Rev. A 93, 021601, Rapid Communication

- **Hubbard model: Pinning of occupation numbers and role of symmetries (2015)**  
Christian Schilling  
Phys. Rev. B 92, 155149
- **Quasipinning and its relevance for  $N$ -Fermion quantum states (2015)**  
Christian Schilling  
Phys. Rev. A 91, 022105
- **Duality of reduced density matrices and their eigenvalues (2014)**  
Christian Schilling, Rolf Schilling  
J. Phys. A 47, 415305
- **The Quantum Marginal Problem (2014)**  
Christian Schilling  
Mathematical Results in Quantum Mechanics 10, World Scientific
- **Natural Orbitals and Occupation Numbers for Harmonium: Fermions versus Bosons (2013)**  
Christian Schilling  
Phys. Rev. A 88, 042105
- **Pinning of Fermionic Occupation Numbers (2013)**  
Christian Schilling, David Gross, and Matthias Christandl  
Phys. Rev. Lett. 110, 040404  
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