



\langle NUMERIQS \rangle

C02 Hybrid Approaches to Quantum Many-Body Systems

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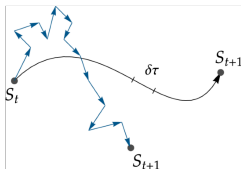
PI & HISKP @ University of Bonn
IAS-4 @ Forschungszentrum Jülich
Max Plank Institute für Kohleforschung

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Different methods across different disciplines have their intrinsic strengths and weaknesses



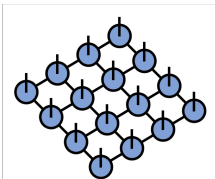
Monte Carlo



Particle physics

- Pros
 - favourable scaling
 - agnostic to form of interaction
 - works in Fock or particular Hilbert spaces
- Cons
 - sign problem
 - ergodicity
 - finite temperature

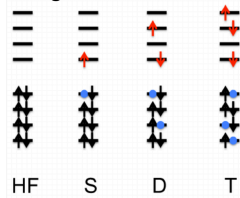
Tensor Network



Condensed matter physics

- Pros
 - no sign problem
 - real-time evolution
- Cons
 - unfavourable scaling
 - finite temperature
 - works best with low-entanglement systems

Configuration Interaction

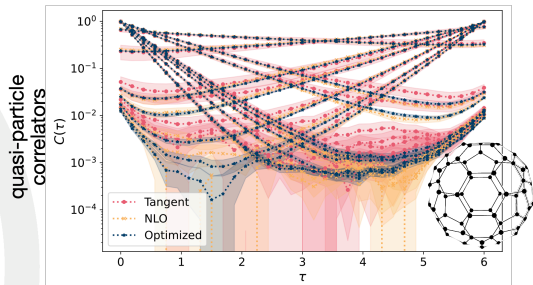
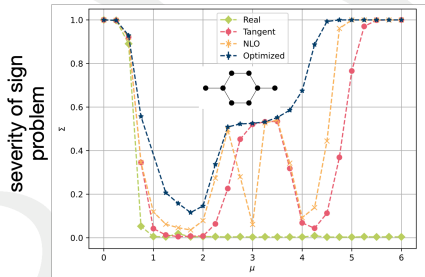
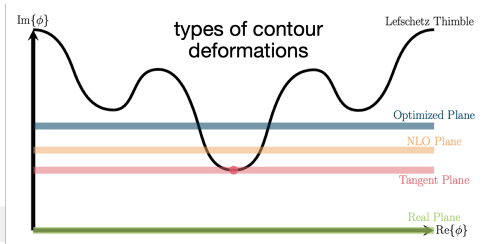


Quantum chemistry

- Pros
 - zero temperature
 - no sign problem
- Cons
 - unfavourable scaling

Tackling the sign problem with contour deformation

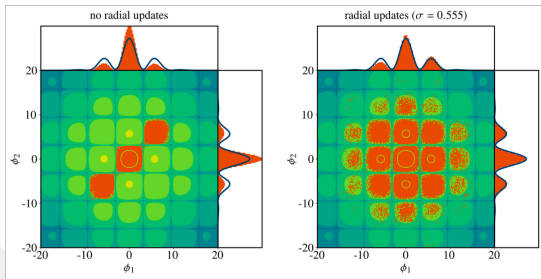
$$\int \mathcal{D}\phi |b\rangle$$



Resolving ergodicity issues



- Simulations of Hubbard model have formal ergodicity problem
- Developed radial updates that jump between topological sectors
 - see F. Temmen's C02 poster
 - see also D. Schuh and J. Kreit's poster related to normalising flows and the Hubbard model

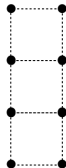
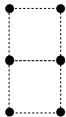


F. Temmen, E. Berkowitz, A. Kennedy, **TL**, J. Ostmeier, X.Yu, *in preparation*

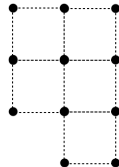
Benchmark systems for all methods



Hubbard model
square lattice

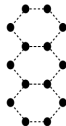


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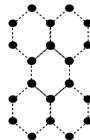


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Hubbard model
hexagonal lattice



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PAH

benzene

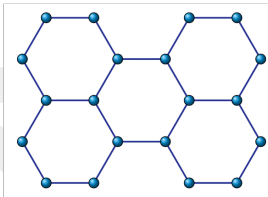
naphthalene

anthracene

perylene

PAH='polycyclic aromatic hydrocarbon'

Spectrum of perylene as a function of doping



M. Rodekamp, E. Berkowitz, C. Gäntegen, Stefan Krieg, TL, J. Ostmeyer, & G. Pederiva [arXiv:2406.06711]

