

Classical benchmarks for variational quantum eigensolver simulations of strongly correlated systems

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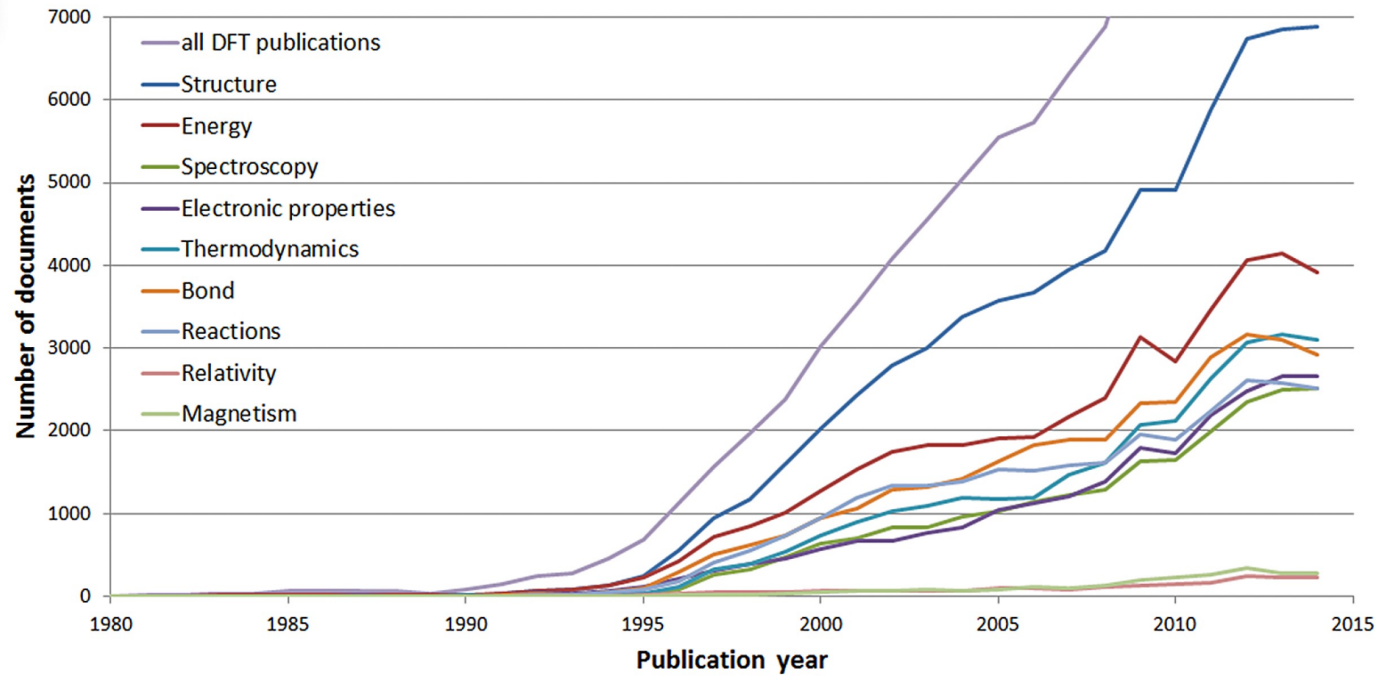
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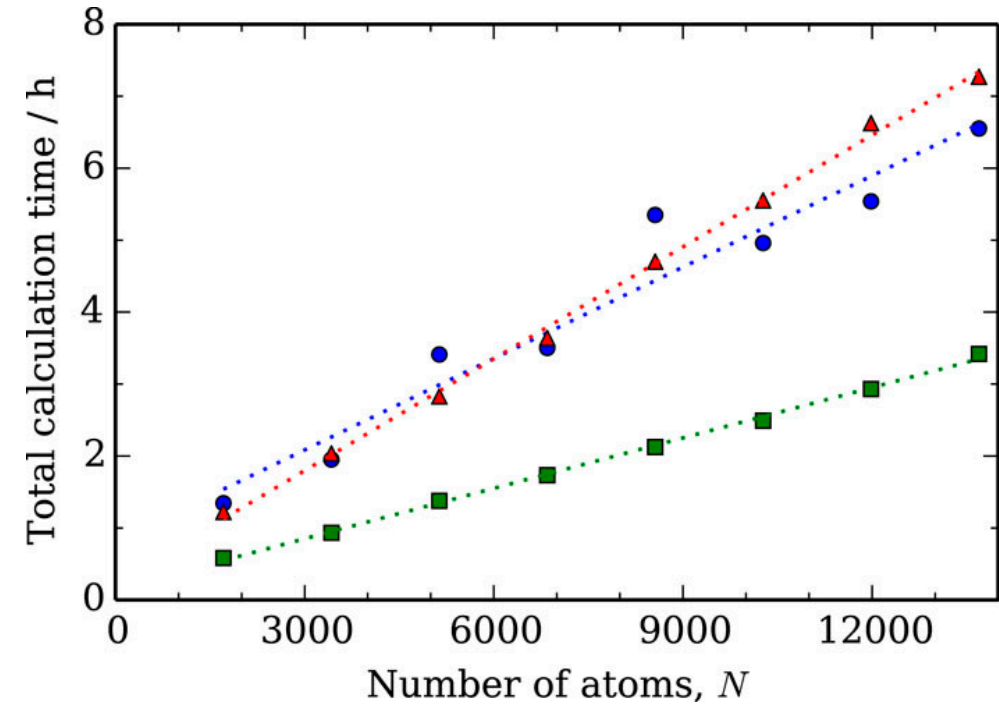
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NQI Joint Algorithms workshop 2024

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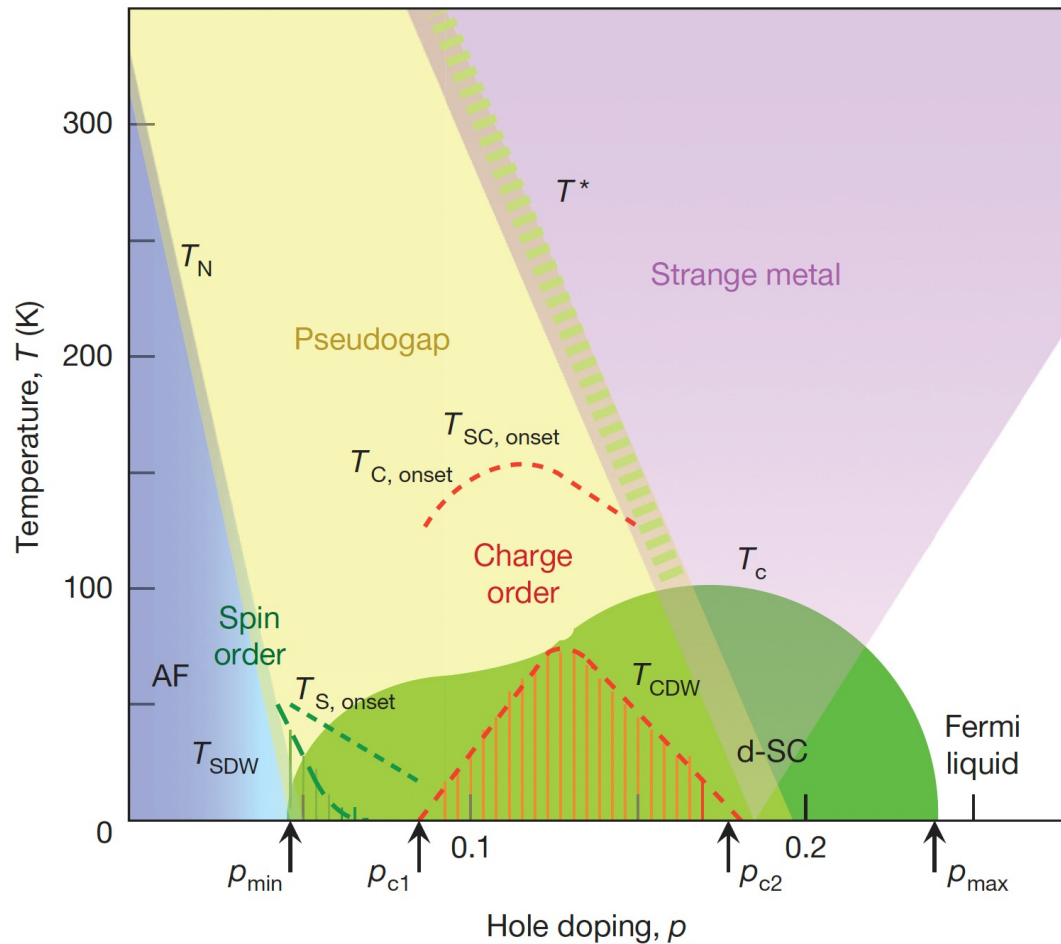


Haunschild *et al.* J Cheminform (2016) 8:52



Prentice *et al.* J. Chem. Phys.. 2020;152(17)

Phase diagram, cuprate high-temperature superconductors



Keimer *et al.* Nature, 518, 179 (2015)

Explicit state of N orbitals:

$$|x_1 x_2 \dots x_N\rangle \longrightarrow 2^N \text{ configurations}$$

For $N = 100$, we have 2^{100} configurations to represent on a classical machine

On quantum hardware, it would in principle suffice to have 100 qubits

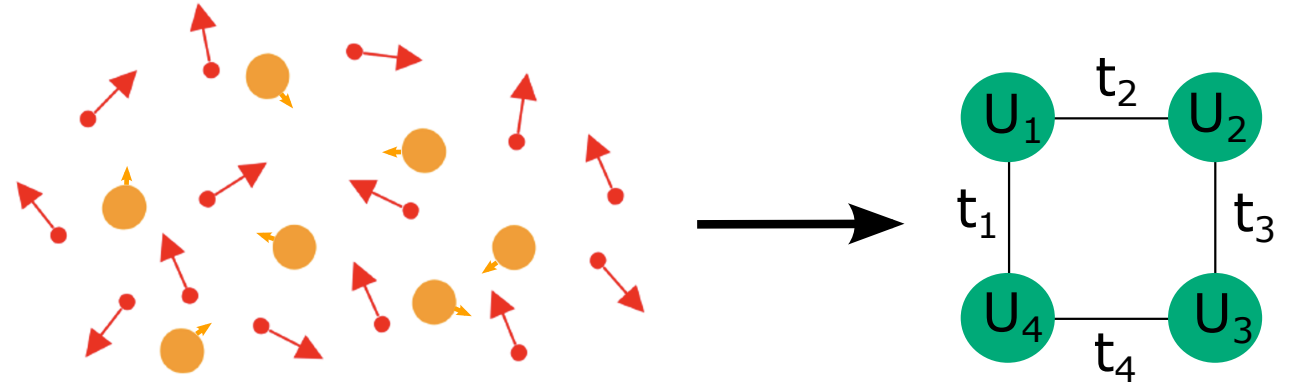
Ab initio downfolding on many-body Hamiltonians

First-principles derivation of extended multi-band Hubbard models within an active space of interest:

$$H = \sum_{\sigma} \sum_{\mathbf{R}\mathbf{R}'} \sum_{ij} t_{i\mathbf{R}j\mathbf{R}'} a_{i\mathbf{R}}^{\sigma\dagger} a_{j\mathbf{R}'}^{\sigma} + \frac{1}{2} \sum_{\sigma\rho} \sum_{\mathbf{R}\mathbf{R}'} \sum_{ij} U_{i\mathbf{R}j\mathbf{R}'} a_{i\mathbf{R}}^{\sigma\dagger} a_{j\mathbf{R}'}^{\rho\dagger} a_{j\mathbf{R}'}^{\rho} a_{i\mathbf{R}}^{\sigma},$$

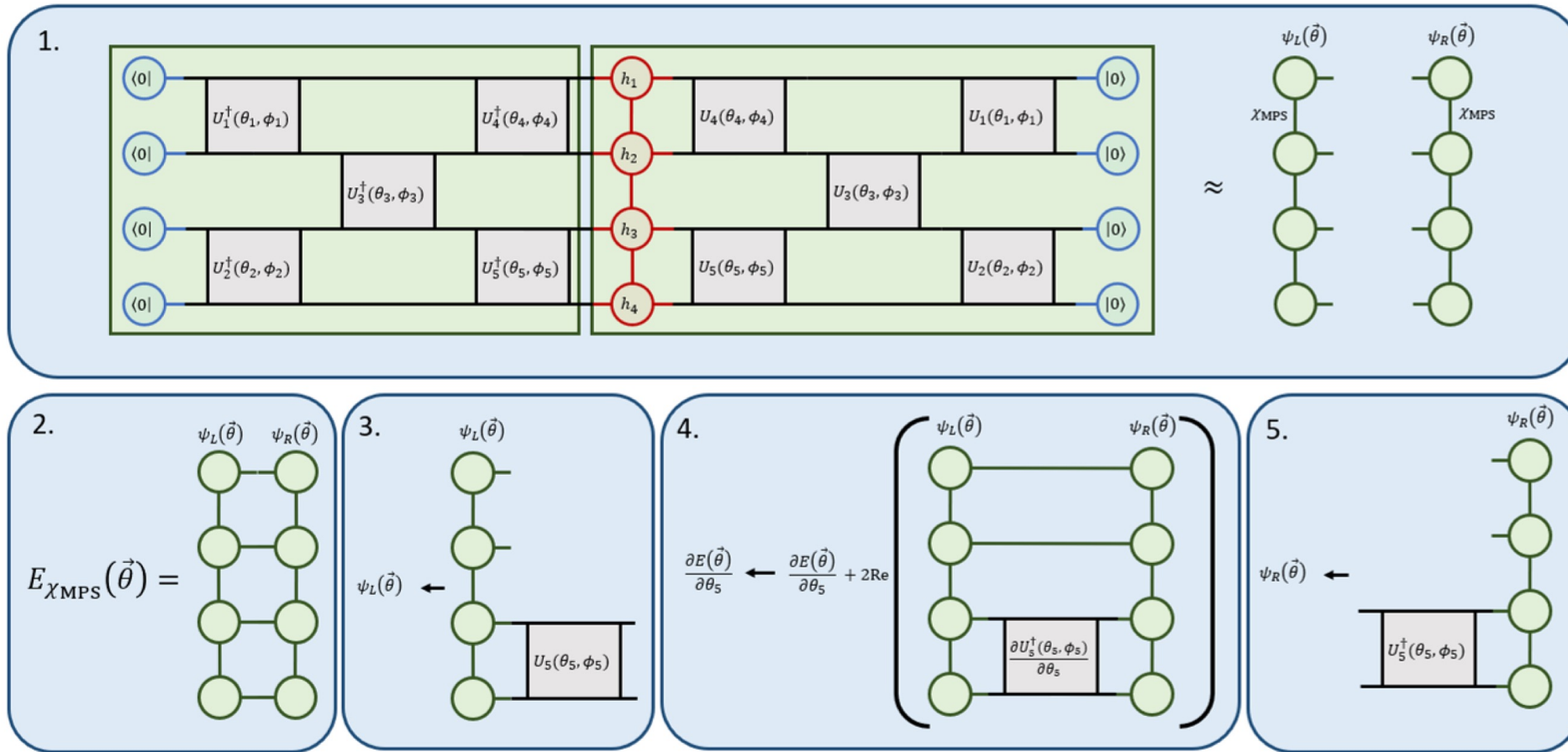
Electronic bands: i, j

Site-localized representation ($\mathbf{R}$),
using Wannier functions



Related codes and approaches:

Zheng et al. *Frontiers in Physics* 6, 2018
Nakamura *et al.* *Comp. Phys. Comm.* 261, 107781, 2021
Romanova *et al.* *npj Comp. Mater.* 9:126, 2023



Khan, Clark, Tubman
arXiv:
2310.12965 (2023)

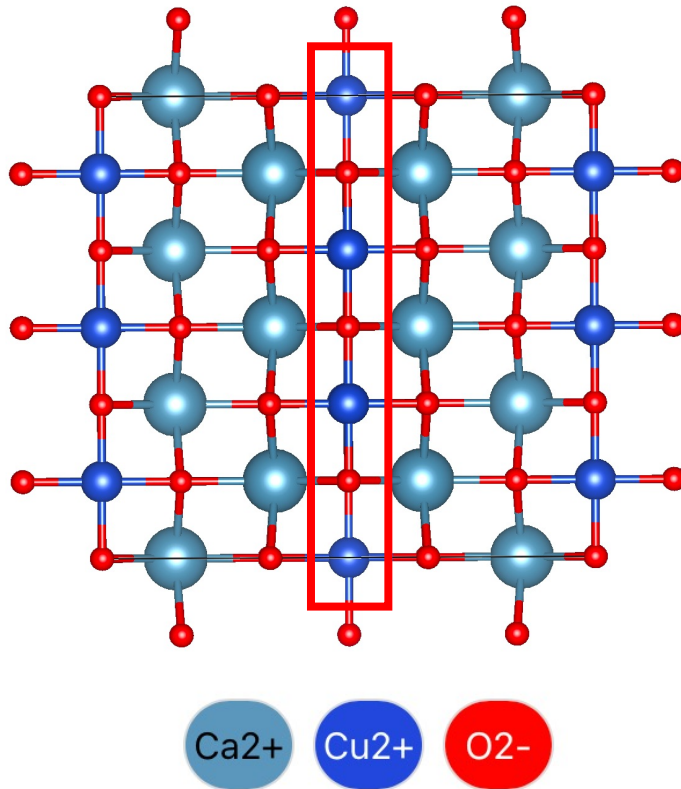
Matrix product state representation of a parametrized quantum circuit:

$$|\psi_{\text{PQC}}(\vec{\theta})\rangle = U_n(\vec{\theta}_n) \dots U_2(\vec{\theta}_2) U_1(\vec{\theta}_1) |\psi_0\rangle$$

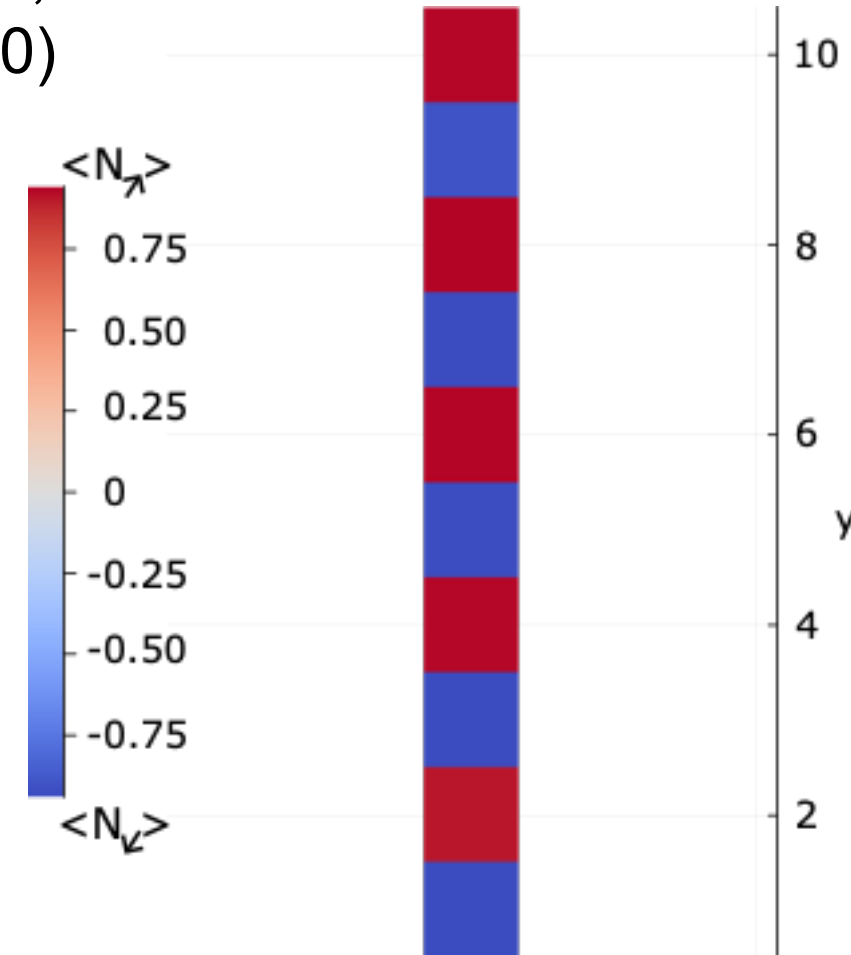
Classically optimize the energy function: $E_\chi(\vec{\theta}) = \langle \psi_\chi(\vec{\theta}) | H | \psi_\chi(\vec{\theta}) \rangle$

Quasi-1D cuprate material: Ca_2CuO_3 and antiferromagnetism

Ca_2CuO_3 is a prototypical 1D-antiferromagnetic material, see e.g., Graaf and Illas, Phys. Rev. B 63, 014404 (2000)



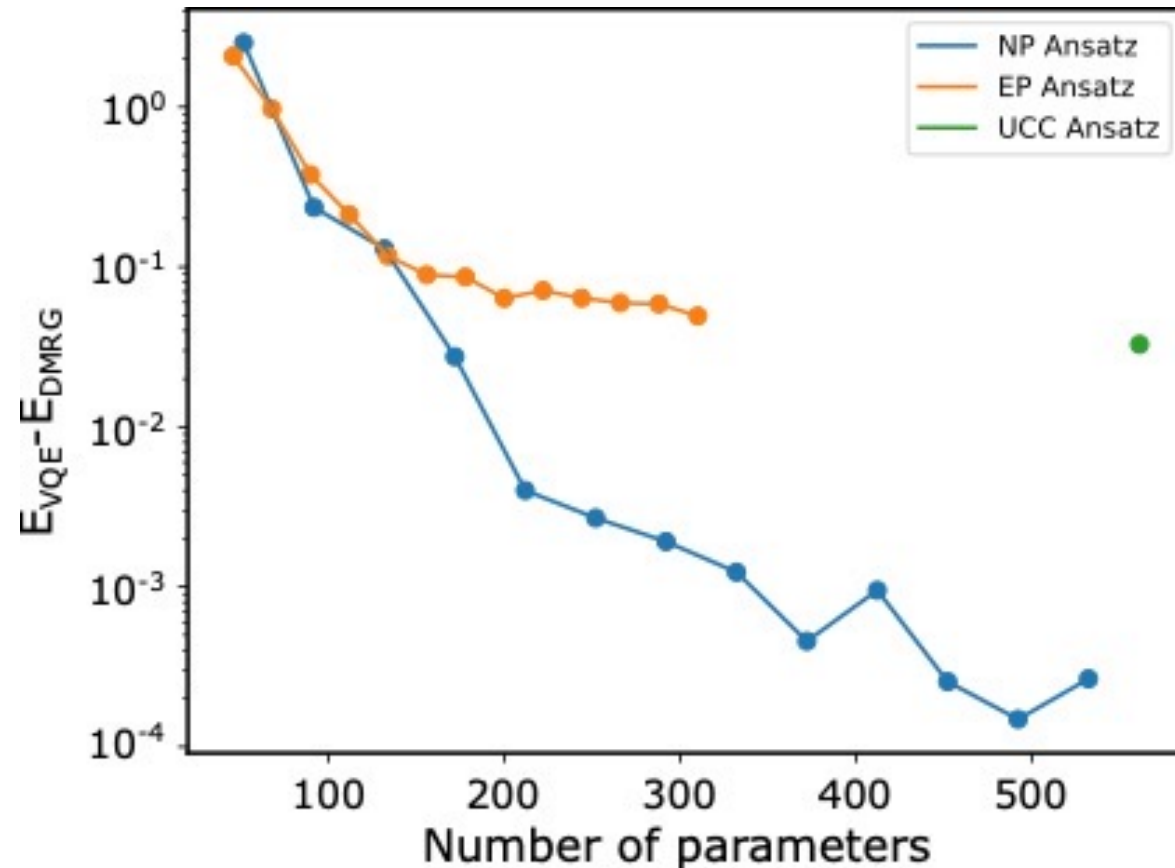
VQE on 1x10 lattice of one-band Hubbard model (20 qubits):



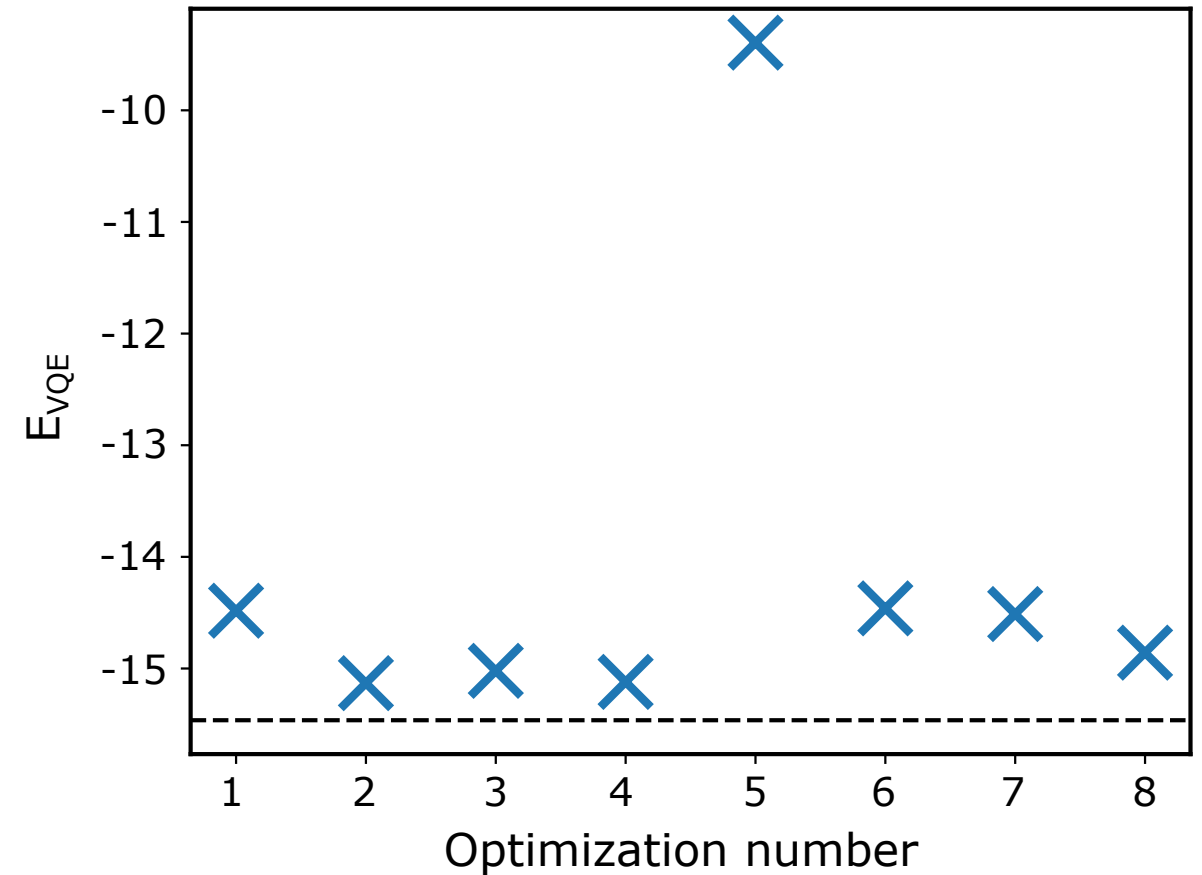
Quantitative classical benchmarking

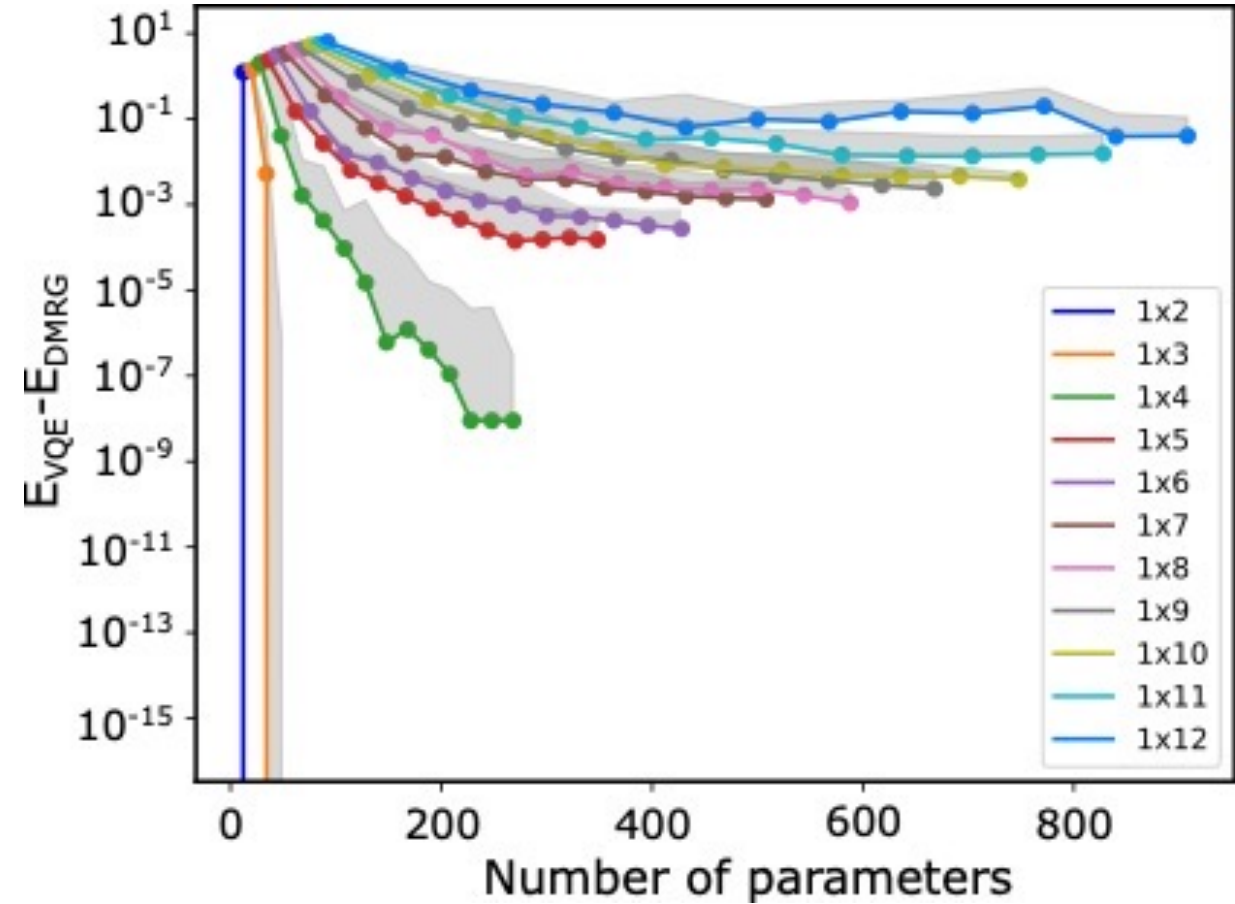
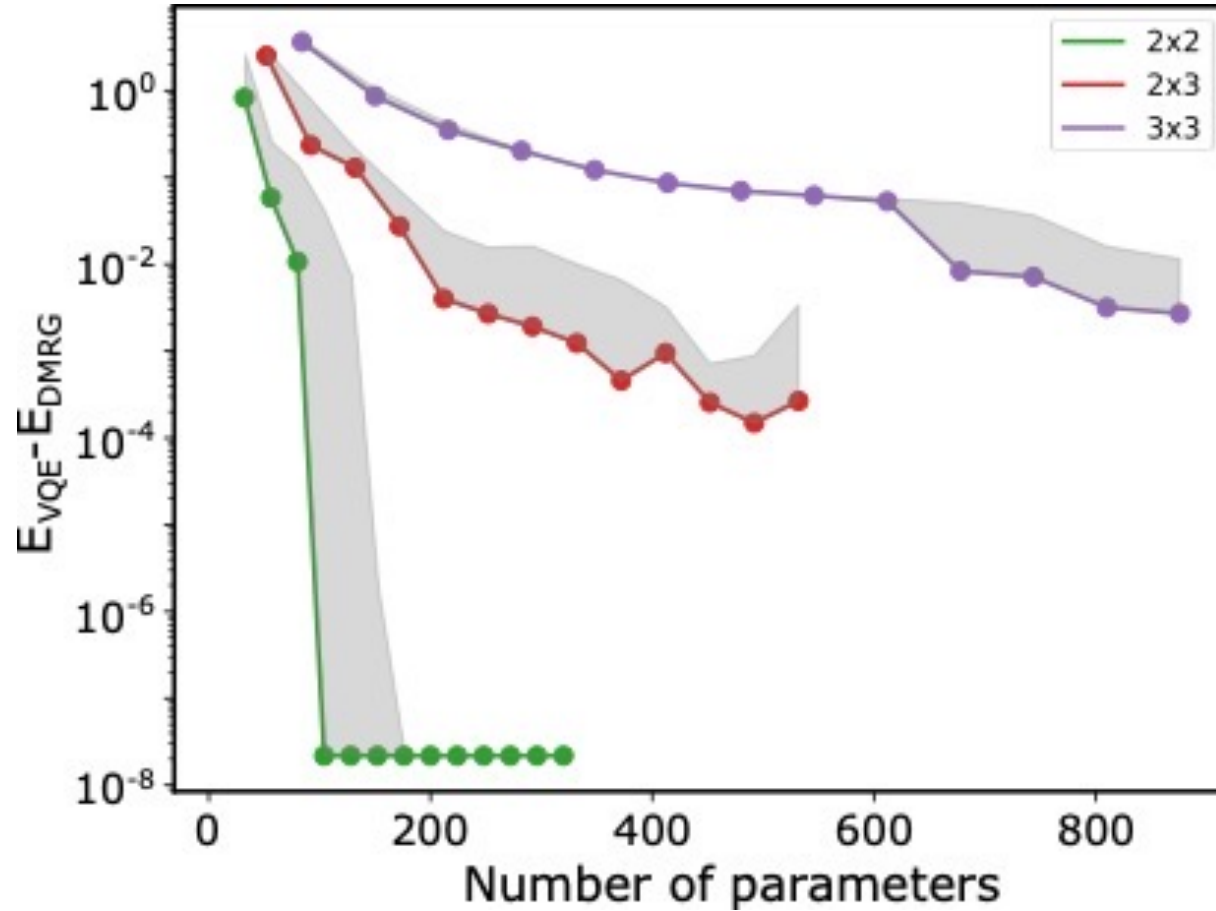
$$H = -t \sum_{\sigma} \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} a_{\mathbf{R}}^{\sigma \dagger} a_{\mathbf{R}'}^{\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R} \uparrow} n_{\mathbf{R} \downarrow}$$

Ansatz comparison (2x3 lattice)

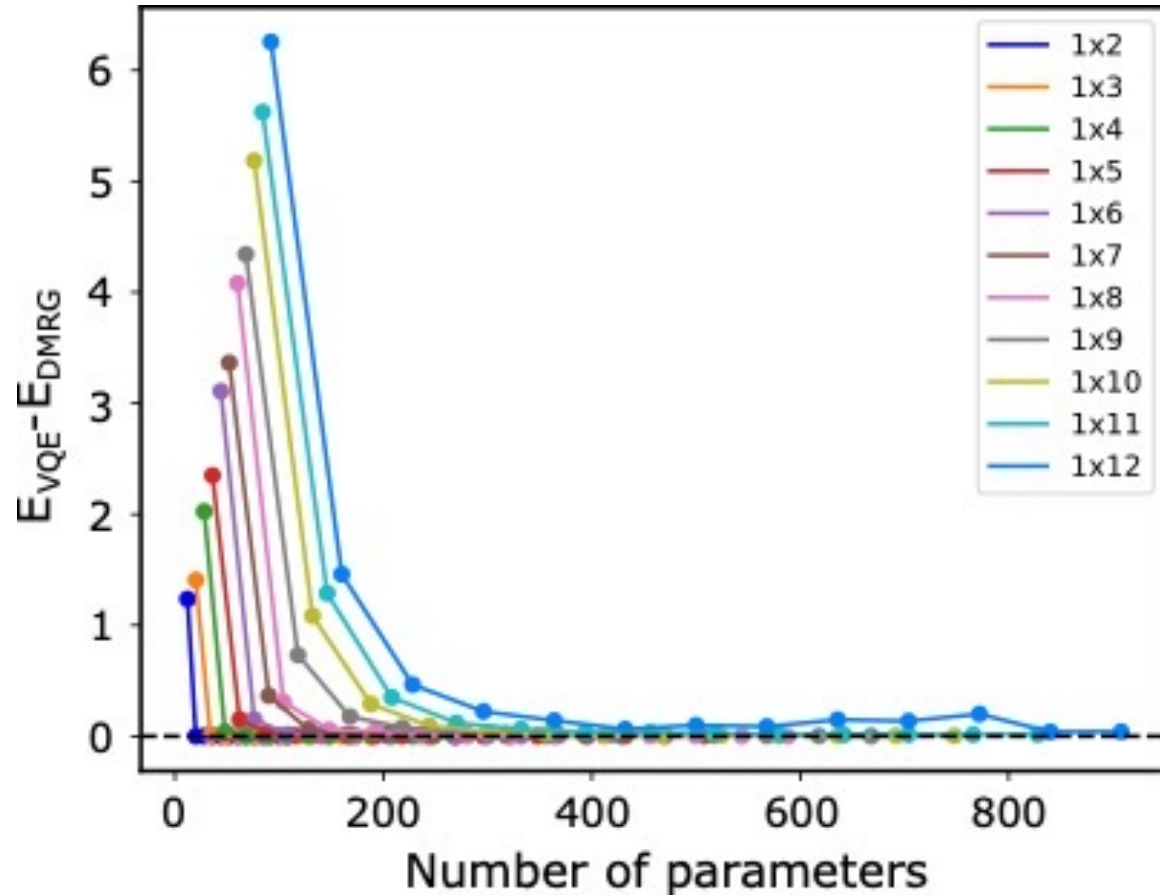


VQE optimizations on 4x4 lattice

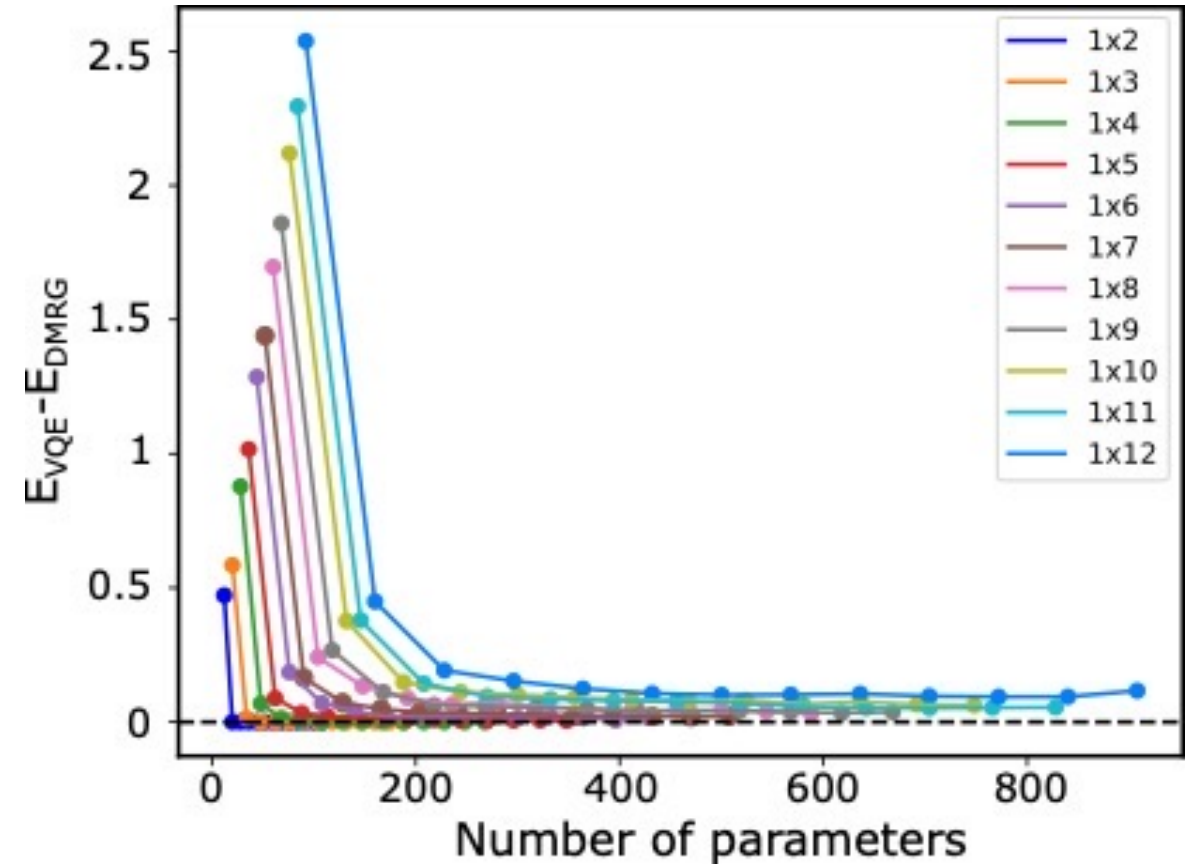




$$\frac{U}{t} = 2$$

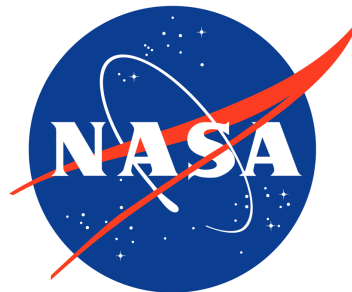


$$\frac{U}{t} = 8$$



Conclusions

- Quantum computers hold promise for the study of electronic structure in strongly correlated materials
- *Ab initio* downfolding rigorous and cost-effective approach to prepare complex systems for quantum simulation
- VQE with current ansatze can yield qualitatively correct ground states for strongly correlated systems
- Ground state energy plateaus for larger lattices and stronger correlations calling for more accurate and flexible approaches as we move towards quantitative accuracy



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