Towards efficient quantum computing for quantum chemistry: reducing circuit complexity with transcorrelated and adaptive ansatz techniques

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Faraday Discussions on Correlated Electronic Structure

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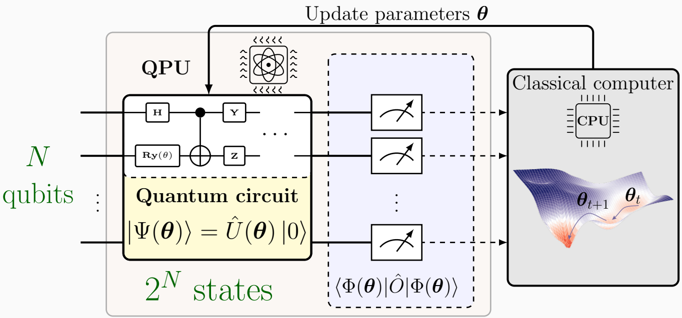
MARIE CURIE ACTIONS

Hybrid Quantum-Classical Approach



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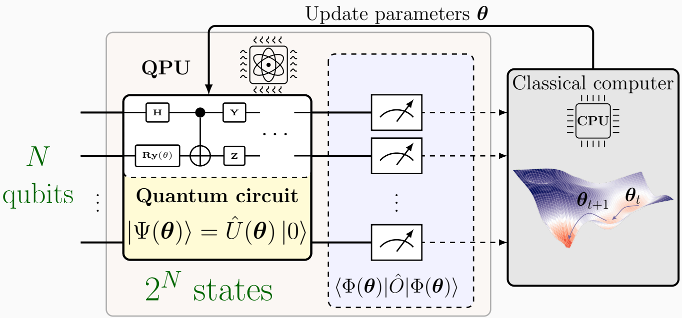


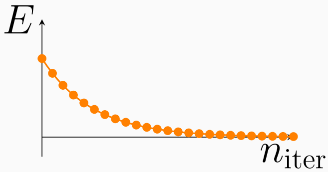
Variational Quantum Eigensolver

$$E(\boldsymbol{\theta}) = \langle\Phi(\boldsymbol{\theta})|\,\hat{H}\,|\Phi(\boldsymbol{\theta})\rangle$$

Quantum Imaginary Time Evolution

for non-Hermitian problems

$$|\Psi_0\rangle = \lim_{\tau\to\infty} \mathrm{e}^{-\hat{H}\tau}\,|\Phi(0)\rangle$$



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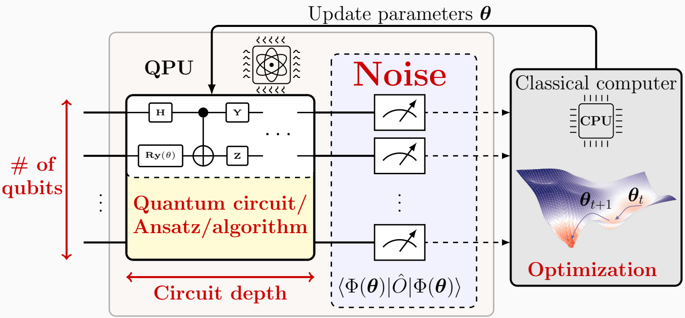

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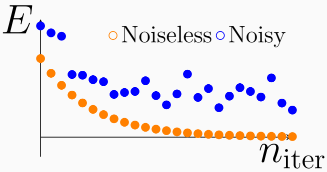
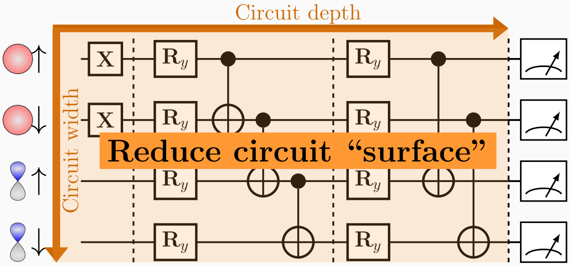


Reduce circuit surface



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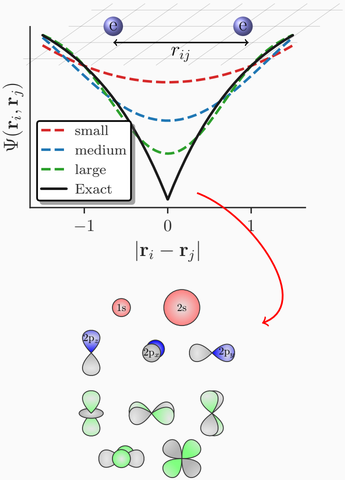

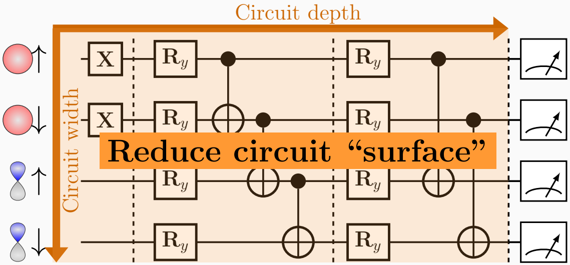

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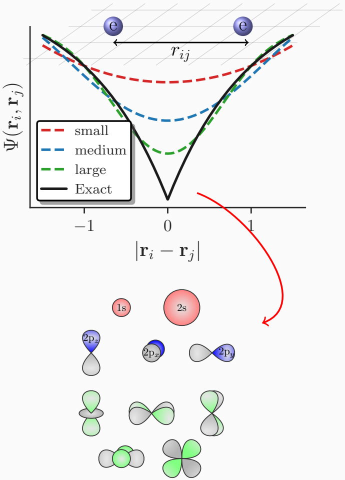
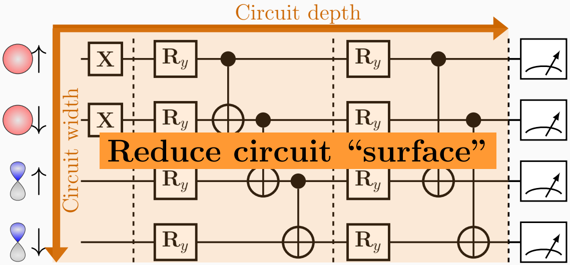
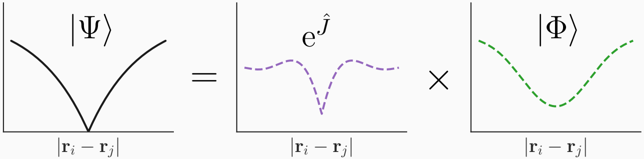




What is the best/shortest Ansatz $\hat{U}(\boldsymbol{\theta})$ to represent $|\Psi_0\rangle$?

ADAPT-ive UCCSD, Grimsley *et al.*, Nat Commun **10**, 3007 (2019)

Explicit correlation – Transcorrelation



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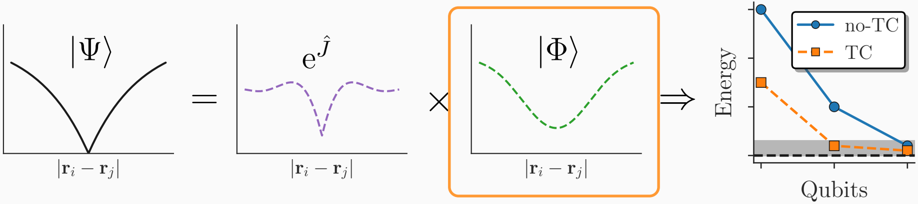

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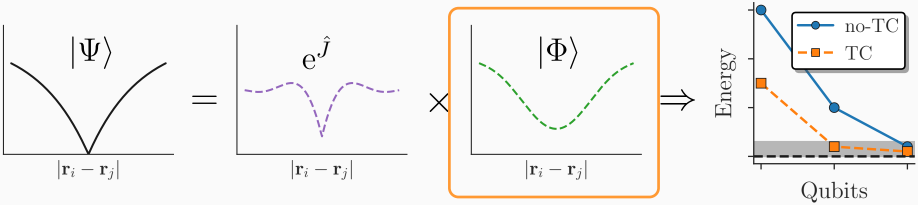

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle \quad \rightarrow \quad |\Psi\rangle = e^{\hat{J}}\,|\Phi\rangle \quad \rightarrow \quad \overbrace{e^{-\hat{J}}\,\hat{H}\,e^{\hat{J}}}^{\hat{H}_{\mathrm{TC}}}\,|\Phi\rangle = E\,|\Phi\rangle$$

$|\Phi\rangle$ easier to represent with less basis functions and shallower quantum circuits

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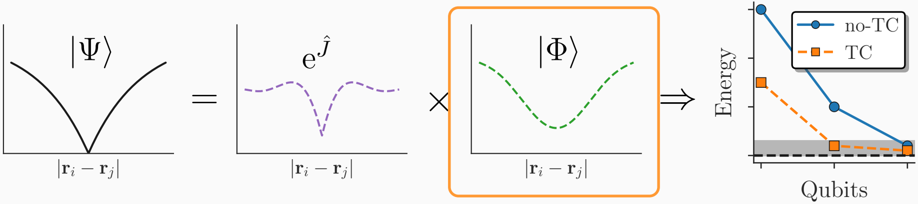

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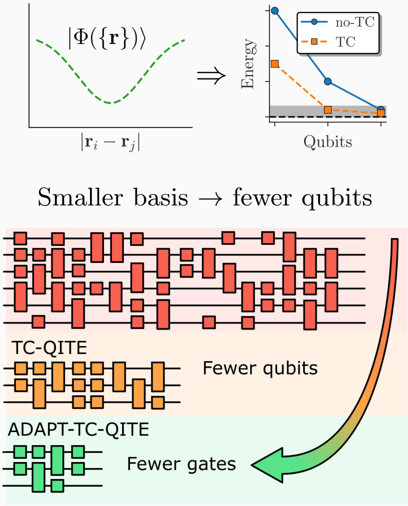
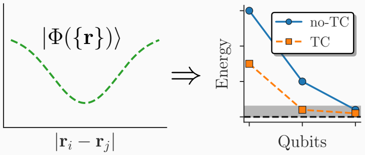
Move complexity from wf. to $\hat{H}_{\mathrm{TC}}$: non-Hermitian* and 3-body terms†

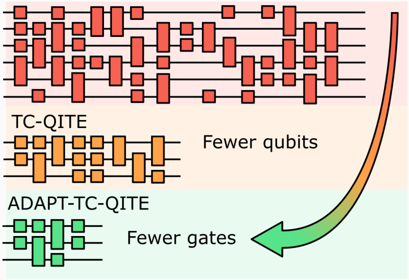
*__TC-VarQITE__, McArdle and Tew, arXiv:2006.11181; __ADAPT-VarQITE__, Gomes *et al.*, Adv. Quantum Technol., **4**, 2100114; †**xTC**, Christlmaier *et al.*, JCP **159**, 014113

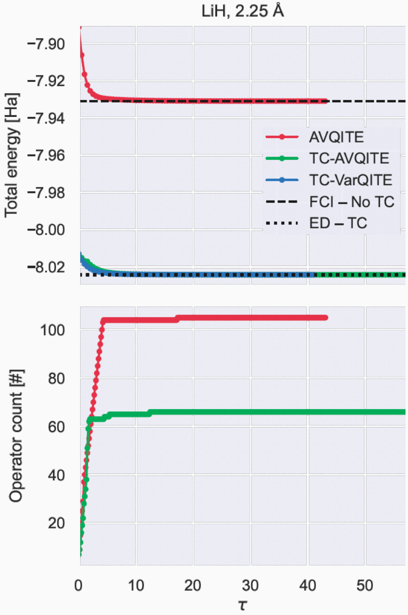


$|\Phi(\{\mathbf{r}\})\rangle$
$|\mathbf{r}_i - \mathbf{r}_j|$
$\Rightarrow$
Energy
no-TC
TC
Qubits
Smaller basis → fewer qubits
TC-QITE
Fewer qubits
ADAPT-TC-QITE
Fewer gates



Smaller basis → fewer qubits





Improved Convergence