

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

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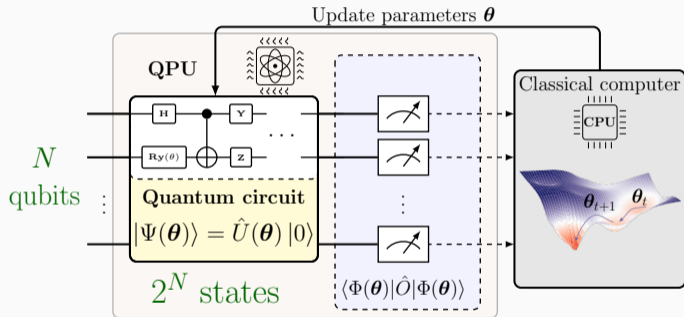
Faraday Discussions on Correlated Electronic Structure



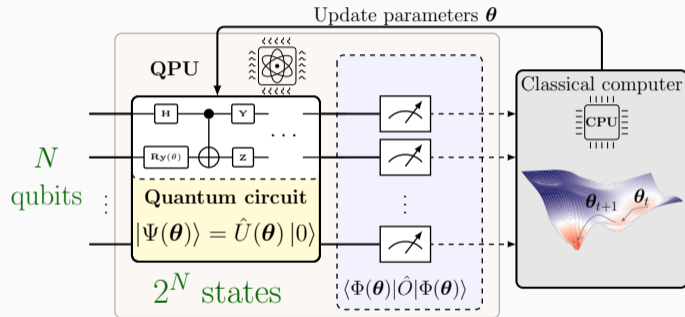
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Hybrid Quantum-Classical Approach



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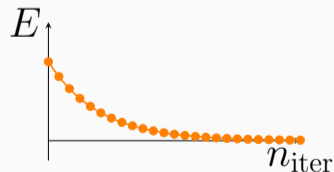
Variational Quantum Eigensolver

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

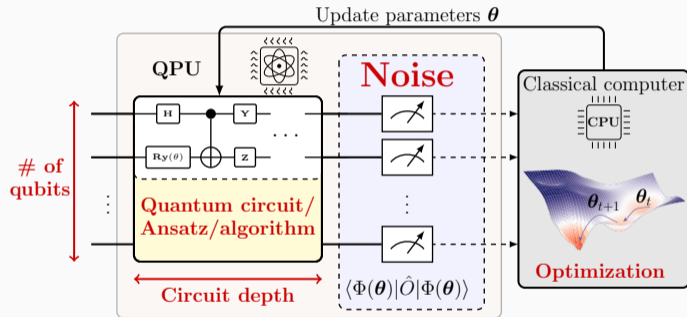
Quantum Imaginary Time Evolution

for non-Hermitian problems

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



Hybrid Quantum-Classical Approach

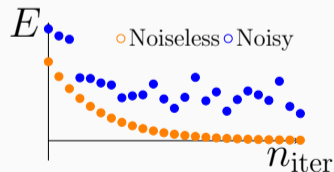


Variational Quantum Eigensolver

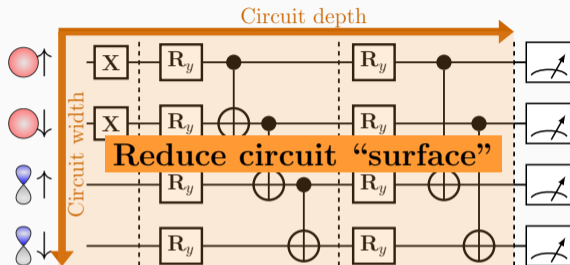
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Quantum Imaginary Time Evolution for non-Hermitian problems

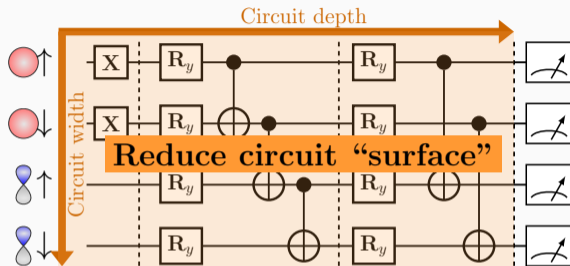
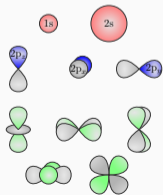
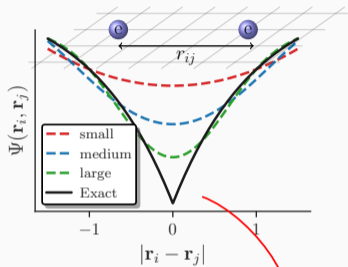
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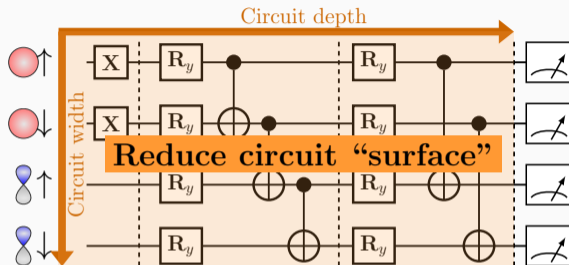
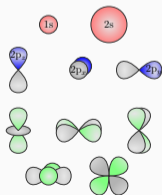
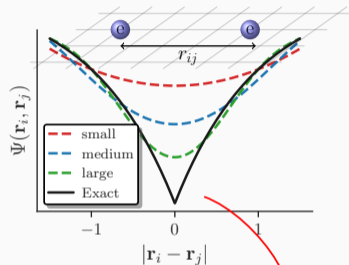
Reduce circuit surface



Reduce circuit surface



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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)

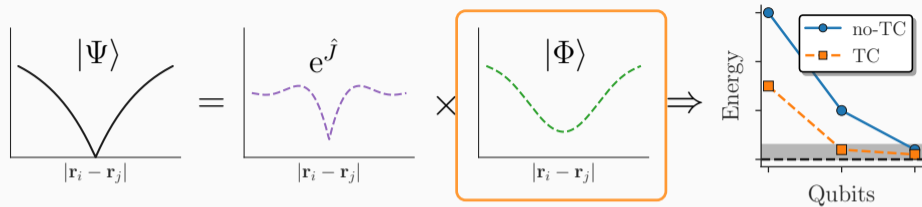
Explicit correlation – Transcorrelation

The diagram illustrates the transcorrelation of a wavefunction. It shows three plots of wavefunctions against the distance $|\mathbf{r}_i - \mathbf{r}_j|$.

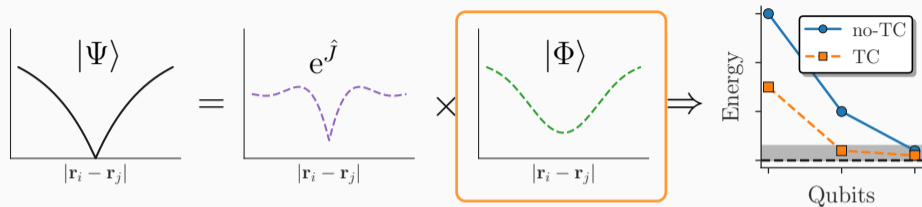
- The first plot shows the ground state wavefunction $|\Psi\rangle$ as a solid black curve with a sharp minimum at the origin.
- The second plot shows the correlation factor $e^{\hat{J}}$ as a dashed purple curve with a sharp minimum at the origin, representing the correlation between the ground state and the reference state.
- The third plot shows the reference wavefunction $|\Phi\rangle$ as a dashed green curve with a smooth minimum at the origin.

The equation is represented as: $|\Psi\rangle = e^{\hat{J}} \times |\Phi\rangle$.

Explicit correlation – Transcorrelation



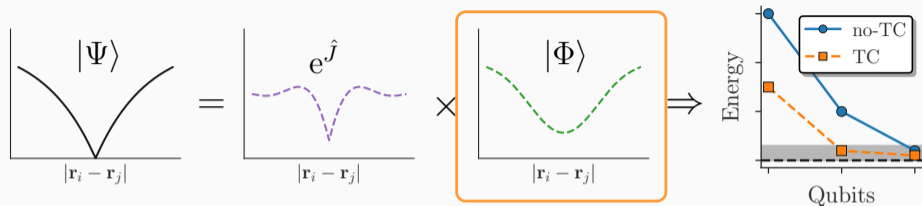
Explicit correlation – Transcorrelation



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

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

Explicit correlation – Transcorrelation

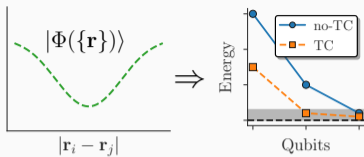


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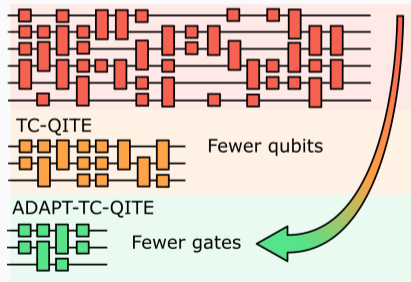
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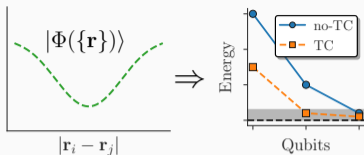
Move complexity from wf. to \hat{H}_{TC} : non-Hermitian* and 3-body terms[†]

***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

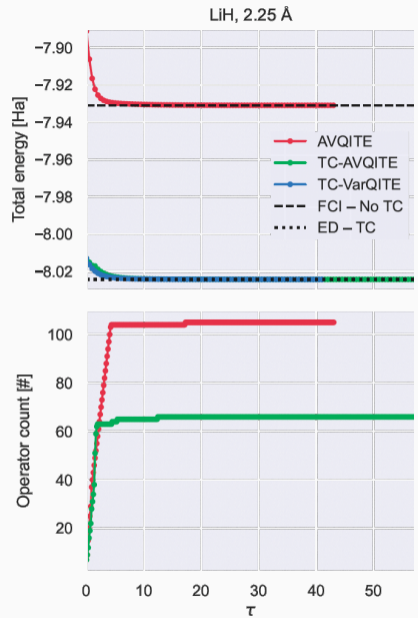
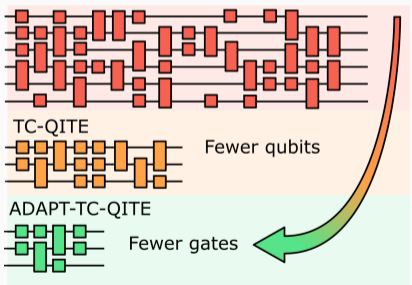


Smaller basis \rightarrow fewer qubits





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Improved Convergence

