Higher order singular-value decomposition for strongly correlated systems

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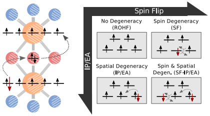
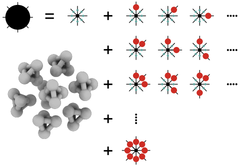
Our group's efforts to model strong correlation

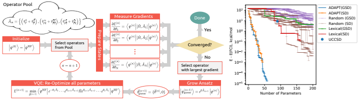
1. Spin-flip-EA-IP methods
    - Strong correlation for spatial/spin near-degeneracies
    - Shannon Houck's talk: COMP 145



2. ***n*-body Tucker approximation**
    - Tensor decomposition
    - Strong correlation for "quasi-clusterable" systems



3. **ADAPT-VQE**
    - Strong correlation for all(?) systems
    - Quantum computation



No Free Lunch Theorem

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- Low-dimensionality
    - DMRG, PEPS, ...
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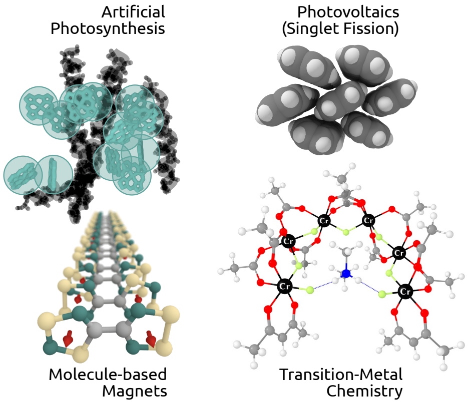
- **“Quasi-Clusterable”**
  - Our focus here



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Artificial

Photovoltaics

Recent methodologcal advances:

- Block-correlated CC (BCCC): Li, JCP, 120, 5017, (2004)
- Renormalized Exciton Method (REM): Al Hajj et al. PRB, 72, 224412, (2005)
- Active-space Decomposition (ASD): Parker, et al. JCP. 139(2), 21108, (2013)
- Ab Initio Frenkel/Davydov Exciton (AIFDEM): Morrison & Herbert. JCTC, 10, 5366, (2014)
- Cluster mean-field (cMF): Jiménez-Hoyos & Scuseria. PRB, 92(8), 85101, (2015)
- excitonic CC (XCC): Lui & Dutoi, arXiv:1709.01966 (2017)

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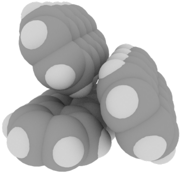

- Imagine a “clusterable” molecular system comprised of 3 clusters,

$$
\begin{aligned}
|\psi\rangle &= C_{ijk} \left|A_i B_j C_k\right\rangle \\
&= C_{\alpha\beta\gamma} U_{i\alpha} U_{j\beta} U_{k\gamma} \left|A_i B_j C_k\right\rangle \quad \text{Tucker Decomposition} \\
&= C_{\alpha\beta\gamma} \left|\tilde{A}_\alpha \tilde{B}_\beta \tilde{C}_\gamma\right\rangle
\end{aligned}
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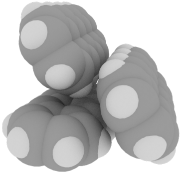
- Working in this compressed space rarely solves the problem - “curse of dimensionality”



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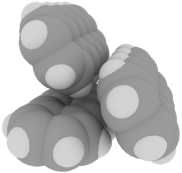

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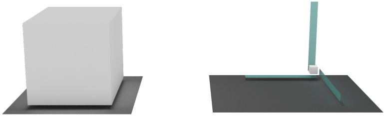
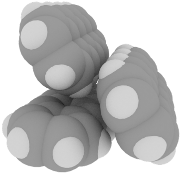


n-body Tucker



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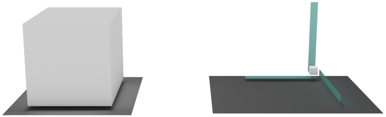

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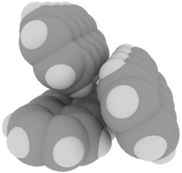

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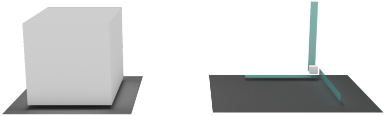

- Define projector onto *important* and *unimportant* vectors for cluster, A:

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- Assume that $\hat{Q}_A$ is "small"

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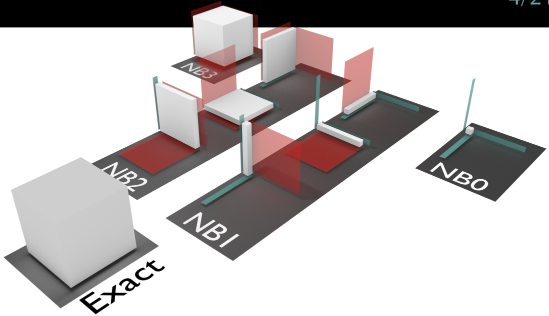

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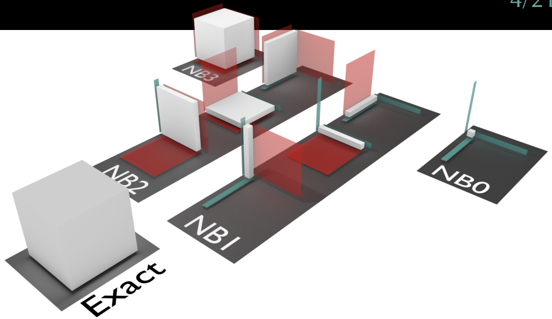

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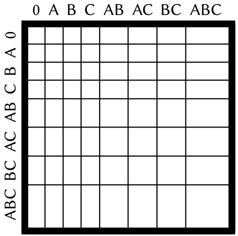

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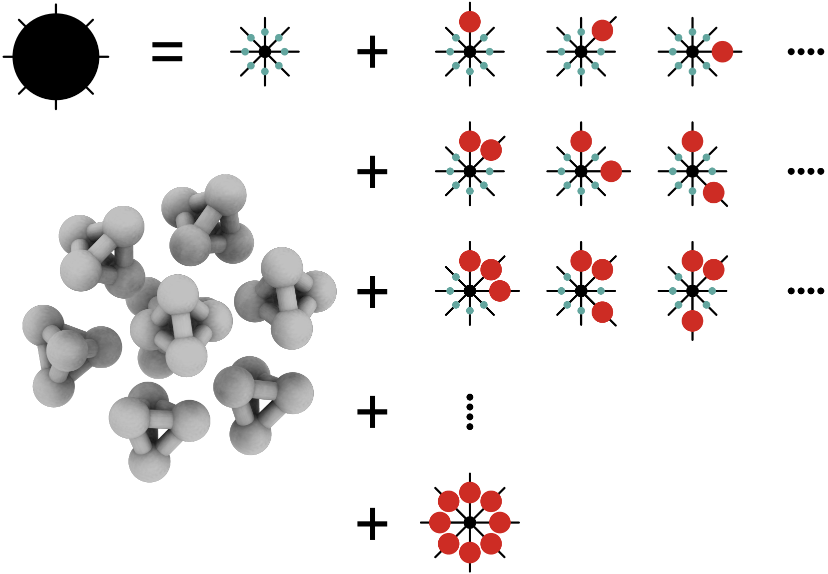
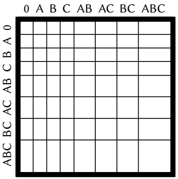


n-body Tucker: direct diagonalization (Heisenberg)



- Heisenberg Hamiltonian implementation
- σ vector elements:

$$\sigma^{k}_{\alpha\beta\gamma} \Leftarrow \left\langle A_\alpha B_\beta C_\gamma \right| \hat{H}_{AB} \left| A_{\alpha'} B_{\beta'} C_{\gamma'} \right\rangle C^{k}_{\alpha'\beta'\gamma'}$$

$$= \sum_{i\in A} \sum_{j\in B} \mathcal{J}_{ij} \left\langle A_\alpha B_\beta \right| \left(\hat{S}^{+}_{i} \hat{S}^{-}_{j} + \hat{S}^{-}_{i} \hat{S}^{+}_{j} + 2\hat{S}^{z}_{i} \hat{S}^{z}_{j} \right) \left| A_{\alpha'} B_{\beta'} \right\rangle \left\langle C_\gamma \middle| C'_\gamma \right\rangle C^{k}_{\alpha'\beta'\gamma'}$$

$$= \sum_{i\in A} \sum_{j\in B} \mathcal{J}_{ij} \left(S^{+}_{i,\alpha\alpha'} S^{-}_{j,\beta\beta'} + S^{-}_{i,\alpha\alpha'} S^{+}_{j,\beta\beta'} + 2S^{z}_{i,\alpha\alpha'} S^{z}_{j,\beta\beta'} \right) C^{k}_{\alpha'\beta'\gamma}$$

$$= H_{\alpha\beta\alpha'\beta'} C^{k}_{\alpha'\beta'\gamma}$$

- The non-interacting Hamiltonian inverse seems to be an effective preconditioner: $\hat{\hat{H}} = \bigoplus_{f} \hat{H}_f$

- Establish self-consistency between Tucker factors and target state
- Two nested optimizations:
  1. Davidson: matrix diagonalization
  2. DIIS: tucker factor optimization
- All quantities computed in the compressed basis
- Davidson gets faster toward end of algorithm

n-body Tucker: Cluster states via HOSVD

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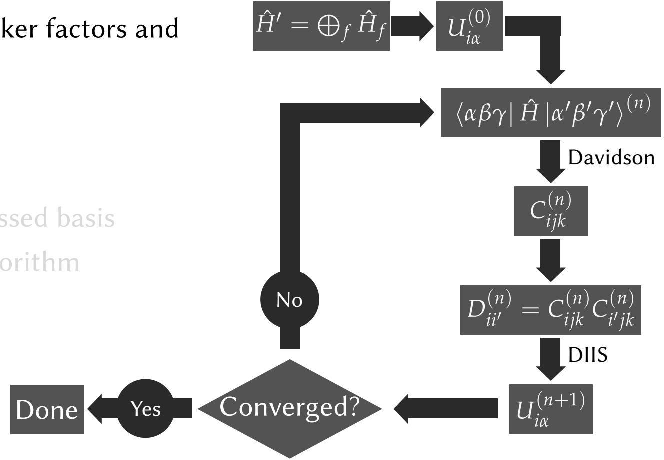

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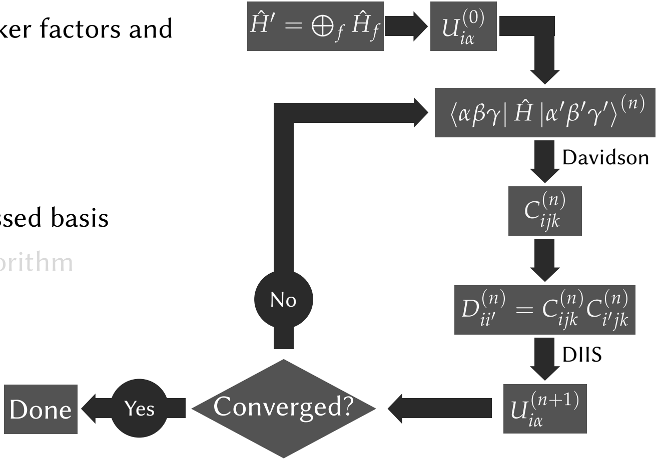

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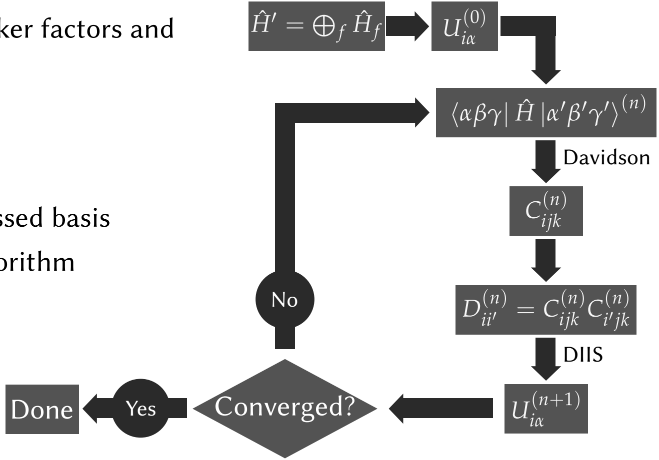
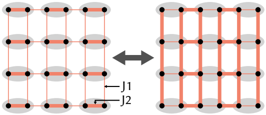


- Clustered Hamiltonian
- Single P vector
- Exponential Convergence
- 4-site clusters
- For single P vector, Tucker optimization nearly negligible



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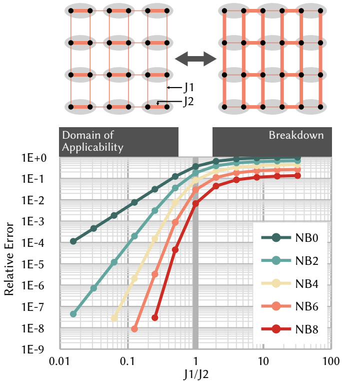

(a) block size = 2

Mayhall, JCTC, 13, 4818 (2017)

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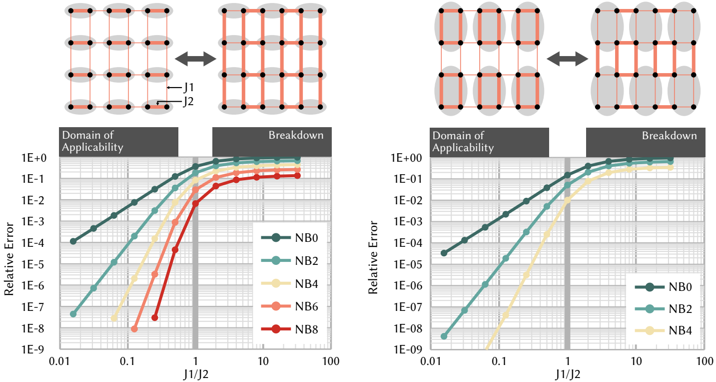

(a) block size = 2 (b) block size = 4

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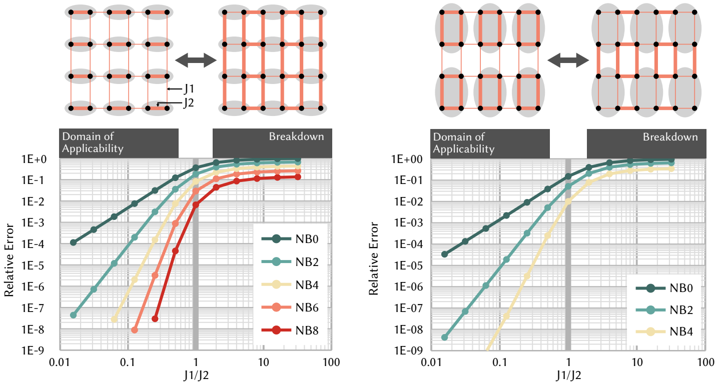

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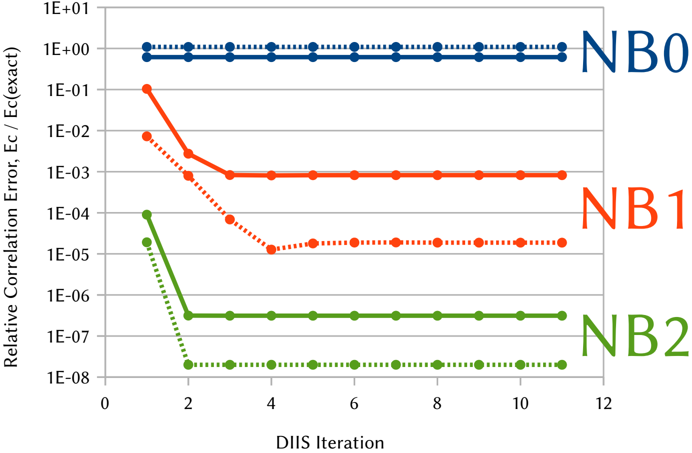
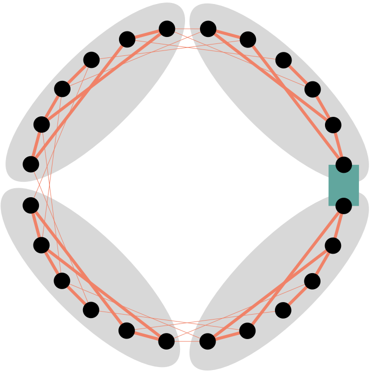
- For multidimensional P spaces, significant benefit from HOSVD

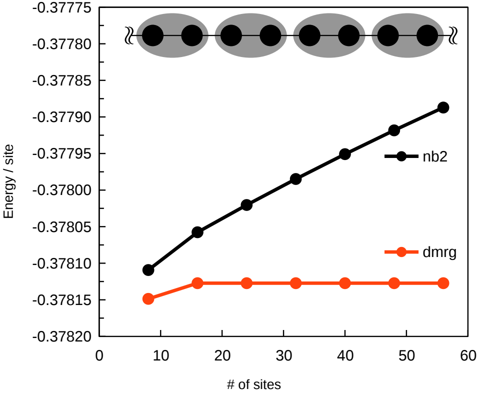




P=(1s+1t)

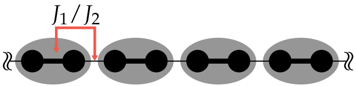
n-body Tucker: Size-extensivity

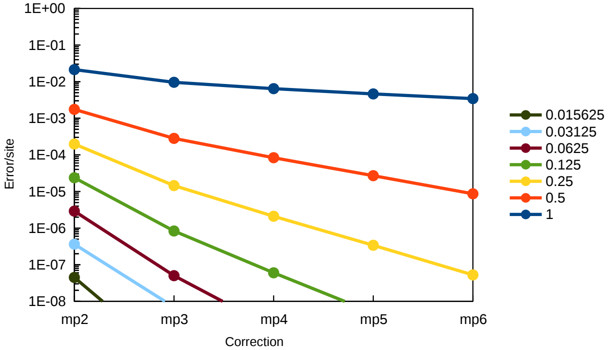
- Compare energy per site to DMRG calculations (ITensor)
- Variational solution not size-extensive



http://itensor.org/about.html

- Higher-order perturbations
- 1D system PBC, thermodynamic limit





n-body Tucker: High order Perturbation theory

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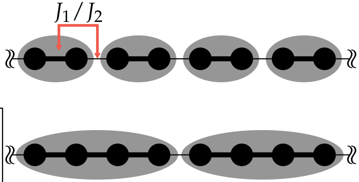
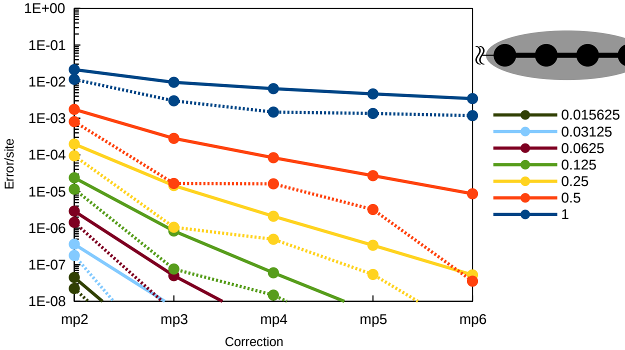
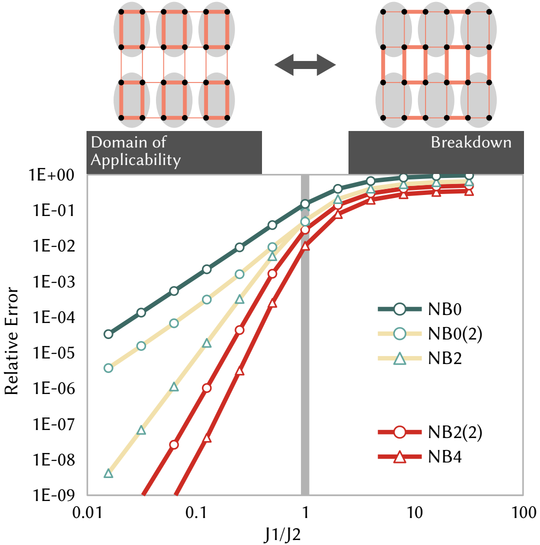




n-body Tucker: CEPA

- A second size-consistant approach: CEPA0-like



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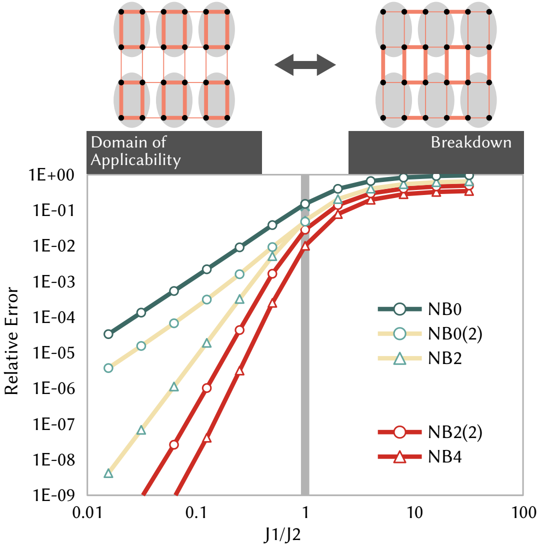
- $\left(\hat{H} - E_0\right) c = 0$
- Identical to D-MBPT(∞) *or* L-CCD



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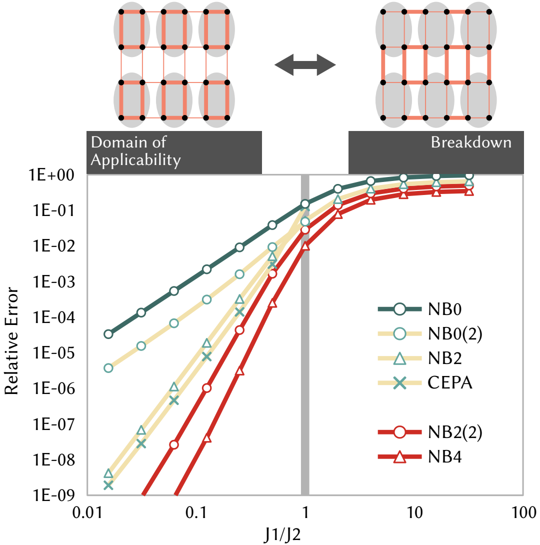
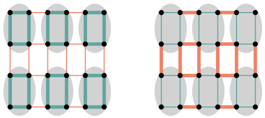
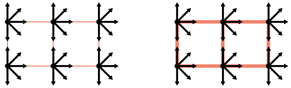
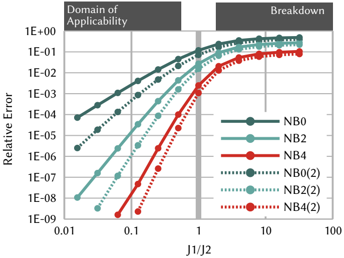
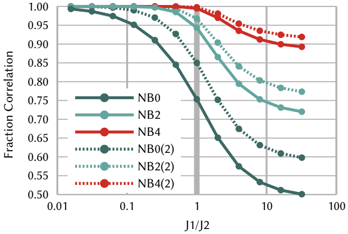


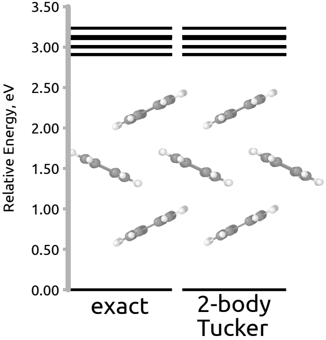
- Magnetic clusters have degenerate groundstates
- Requires larger P space
- n-body terms correct a renormalized spin model



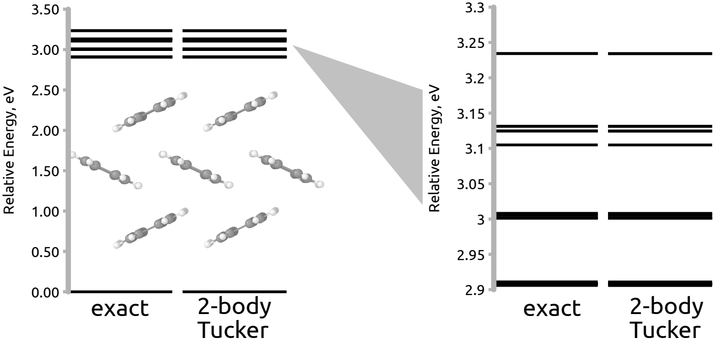








Mayhall, JCTC, 12, 4263 (2016)


3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
Relative Energy, eV
exact
2-body Tucker
3.3
3.25
3.2
3.15
3.1
3.05
3
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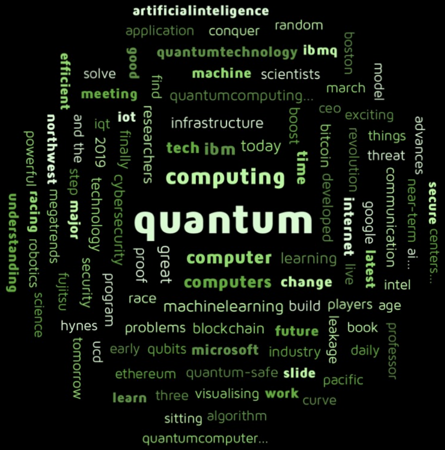
- *Quantum Computation* provide a possible solution



Pulled from #quantumcomputing twitter hashtag

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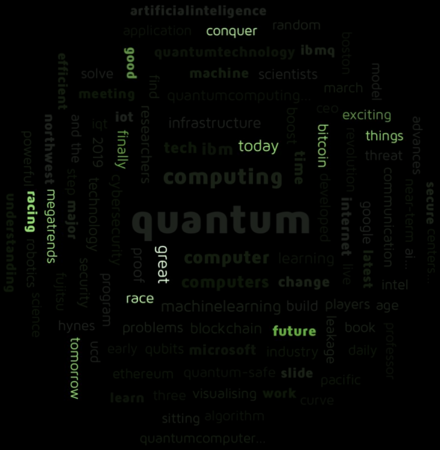
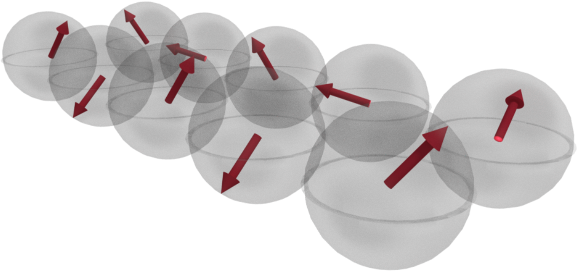


Pulled from #quantumcomputing twitter hashtag

Quantum Computation

- Computational framework comprised of *entangled* quantum bits (qubits)
- **Offensive simplification**: Qubits are “controllable two-level systems”
- Universal quantum computation is quite general
- **Our focus:** simulating quantum systems



- Natural representation of quantum states $\rightarrow$ Computational speedup
- **Classical Computer**: Only represents "classical" basis vectors
    - Store (manipulate) quantum state as vector of numbers in memory
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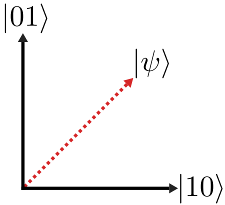
    - Create (measure) quantum state on hardware to mimic simulated quantum state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|10\rangle \pm |01\rangle\right)$$



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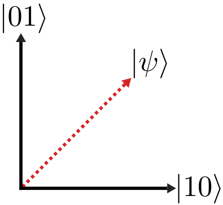

Molecule State		Classical Computer
$\lvert\psi\rangle$	$=$	$\begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$

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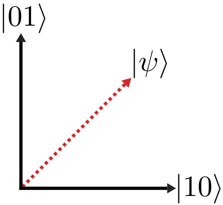

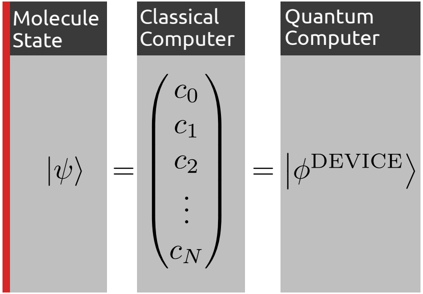

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- Unitary Coupled-Cluster

$$|\psi\rangle = \exp\left\{\sum_i \theta_i \hat{\tau}_i\right\}|0\rangle = \hat{U}(\vec{\theta})\,|0\rangle$$

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$$E(\theta) = \langle \hat{H} \rangle_\theta = \sum_{pq} h_{pq} \left\langle \hat{p}^\dagger \hat{q} \right\rangle_\theta + \sum_{pqrs} \langle pq|rs\rangle \left\langle \hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r} \right\rangle_\theta$$

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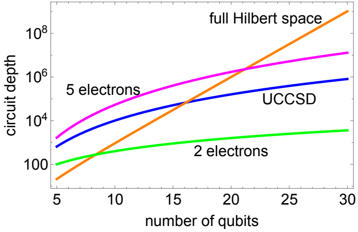

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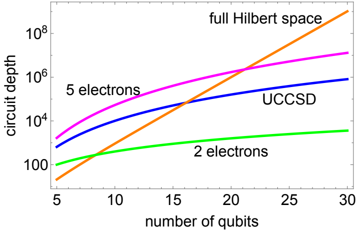

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Grimsley, Economou, Barnes, Mayhall, arXiv:1812.11173 (2018)

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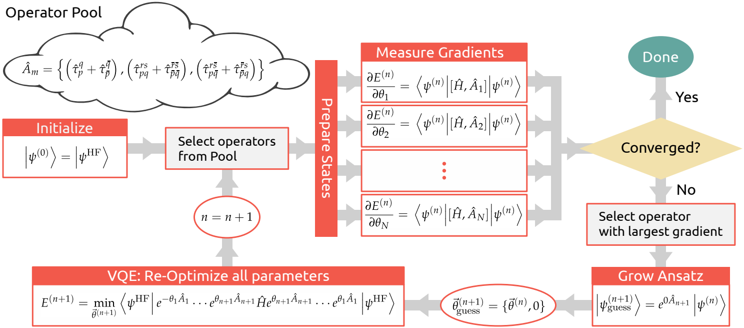

- BeH_2 at $2R_{eq}$ with STO-3G
- Extremely fast convergence with number of parameters!

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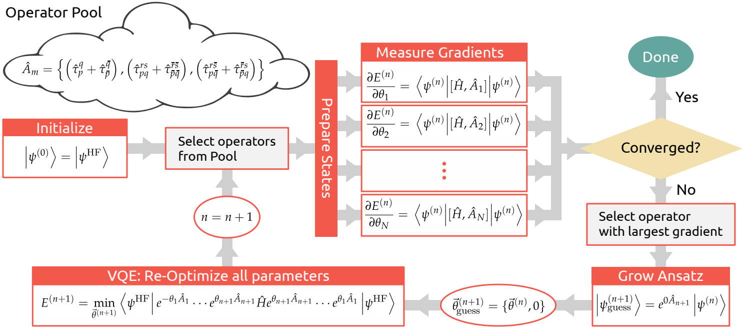
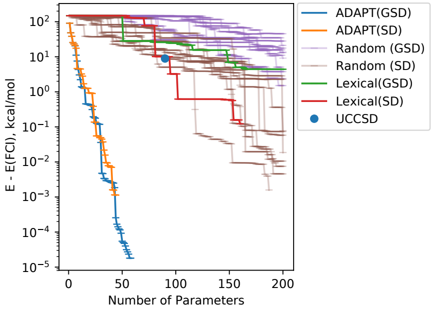
ADAPT-VQE: Algorithm





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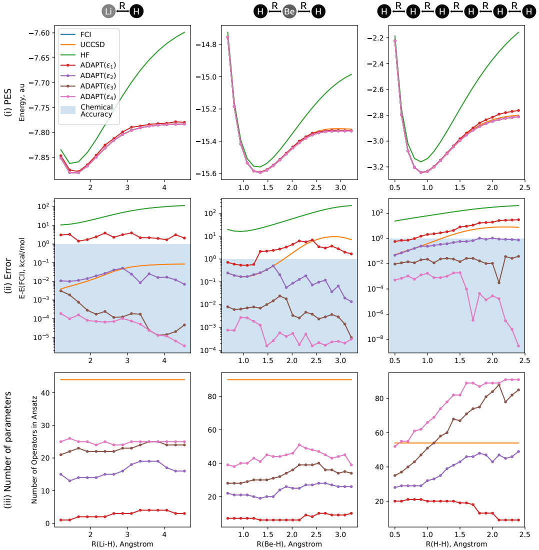
ADAPT-VQE: Potential Energy Curves



(a) LiH dissociation (b) BeH_2 dissociation (c) H_6 dissociation

Grimsley, Economou, Barnes, Mayhall, arXiv:1812.11173 (2018)

Acknowledgements

Students
- Shannon Houck
- Vibin Abraham
- Harper Grimsley
- Robert Smith

Postdocs
- Daniel Claudino
- Oinam Meitei

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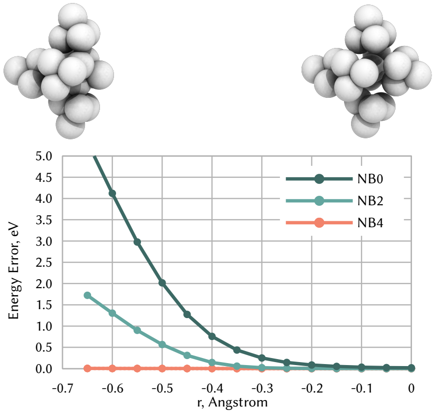
- Sophia Economou (VT Physics)
- Ed Barnes (VT Physics)
- Kyungwha Park (VT Physics)
- Dave Pappas (NIST/UC Boulder)

Funding
- NSF CAREER: 1752612
- DOE: DE-SC0018326
- DOE: DE-SC0019199
- NSF: 1839136

Postdoc and graduate student positions available!

- Convergence of self-consistent “Tucker basis”



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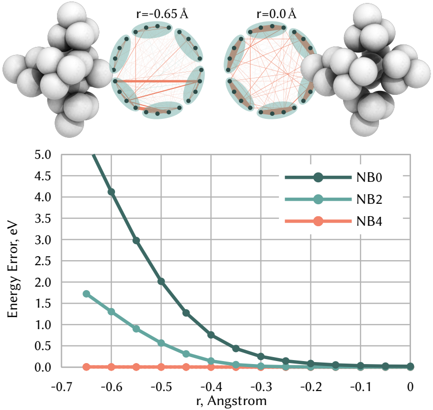

n-body Tucker: self-consistency

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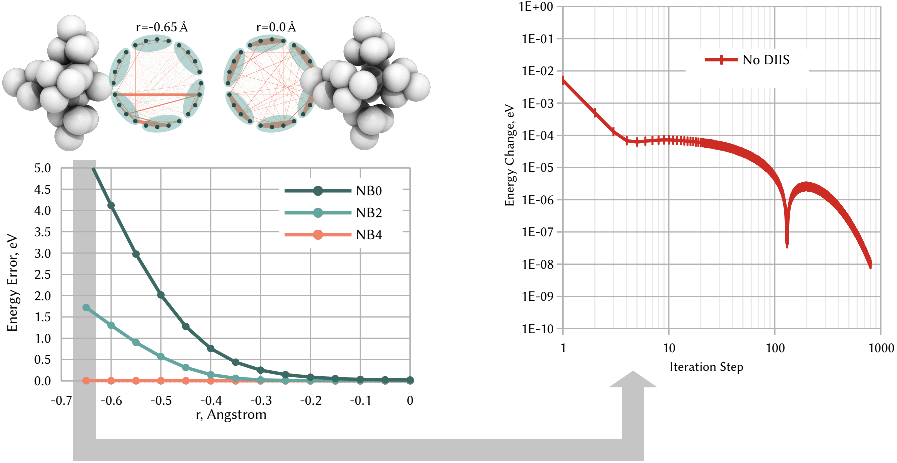

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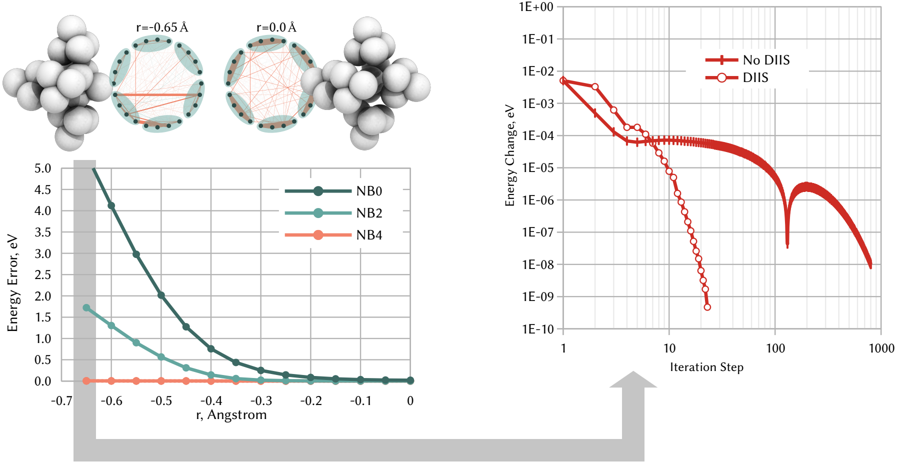

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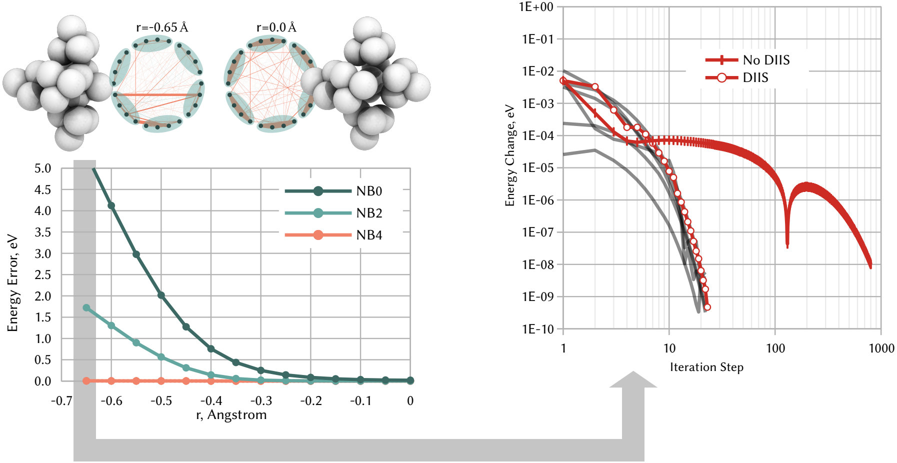
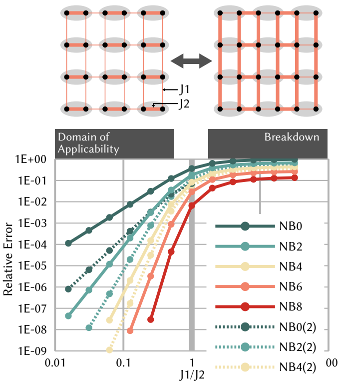
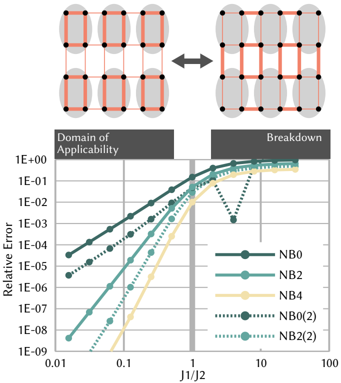


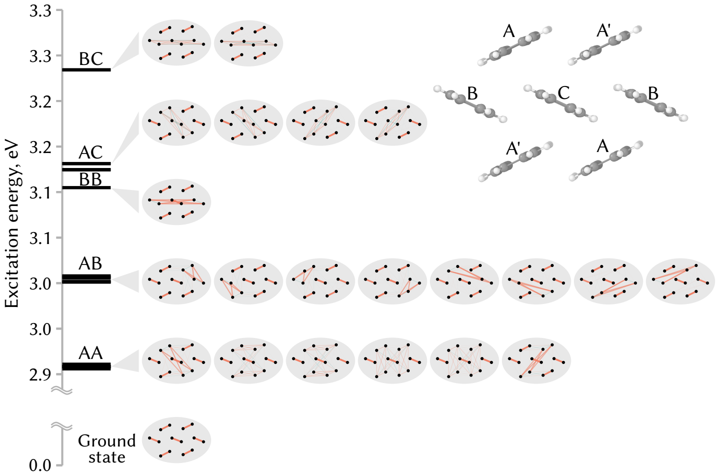
- Perturbation theory via Löwdin Partitioning



(a) block size = 2



(b) block size = 4



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