Observing the Mott Metal-Insulator Transition with Dynamical Mean Field Theory

Speaker: Norman Hogan
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Member of Kemper Lab Research Group

Mathematical Physics Seminar at the University of Iowa
February 27, 2024

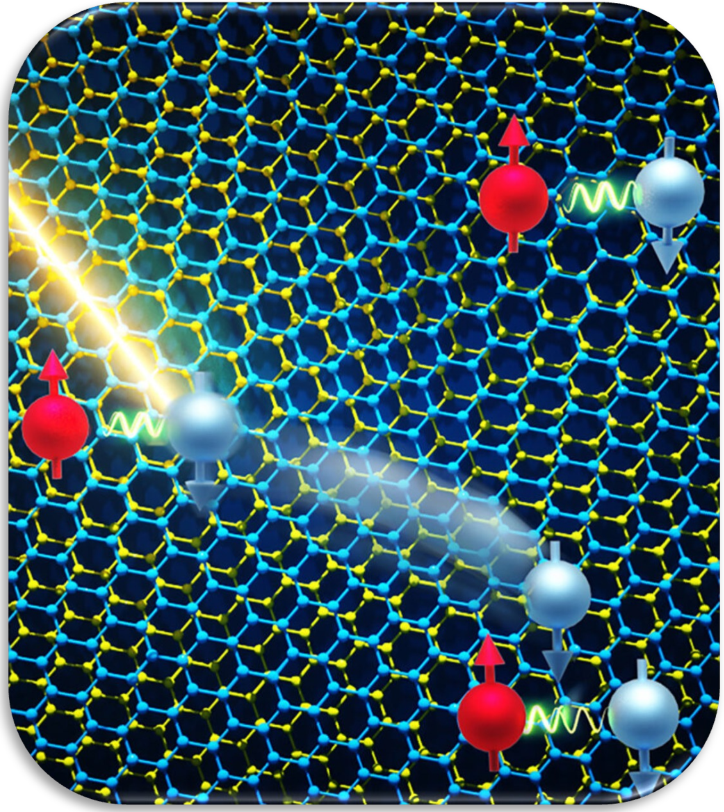

Image: Ella Maru Studio

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- Interacting many-body models
  - One-band Hubbard Model
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- Quantum subspace diagonalization
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  - Preliminary results
- Quantum computation as a tool
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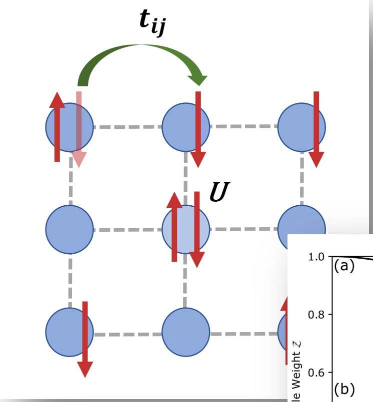

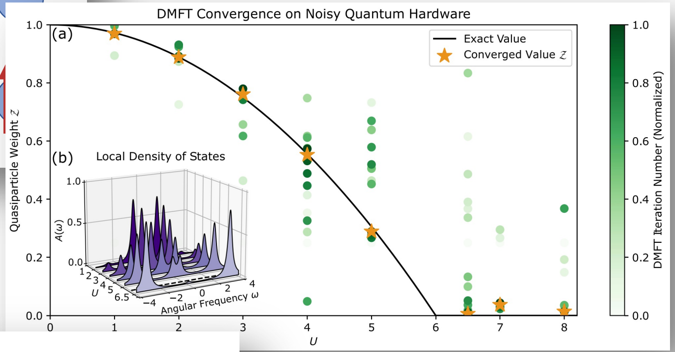

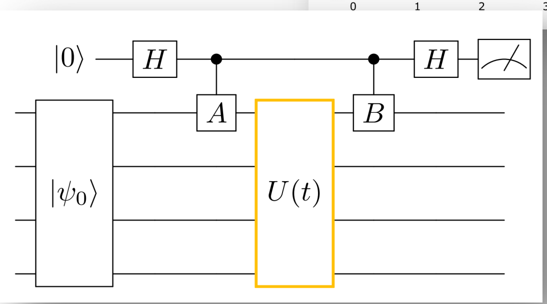

From Steckmann et al.
10.1103/PhysRevResearch.5.023198

Introduction

Why theoretical condensed matter physics?

- To understand many-body systems
  - P.W. Anderson: “More is Different”
- Advancing our knowledge of condensed matter systems leads to advancements in technology
- Solving problems of interest to many fields
  - Materials science
  - Quantum chemistry
  - Computational science

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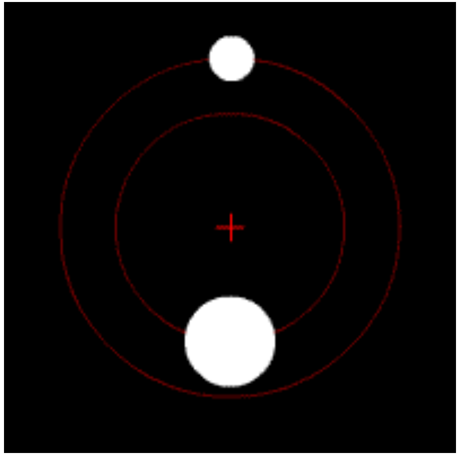

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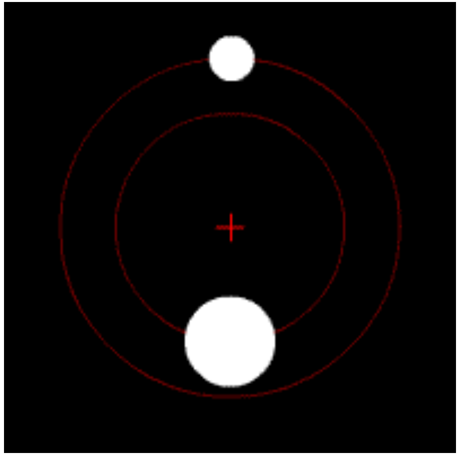

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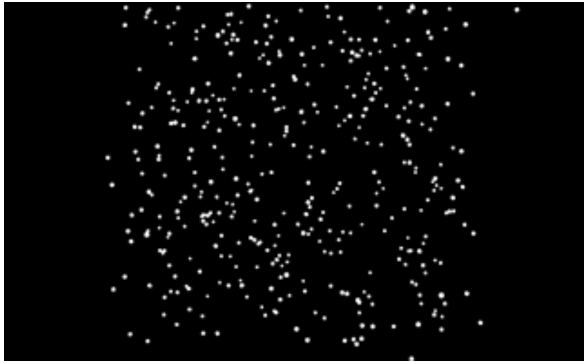

From nbodies on GitHub

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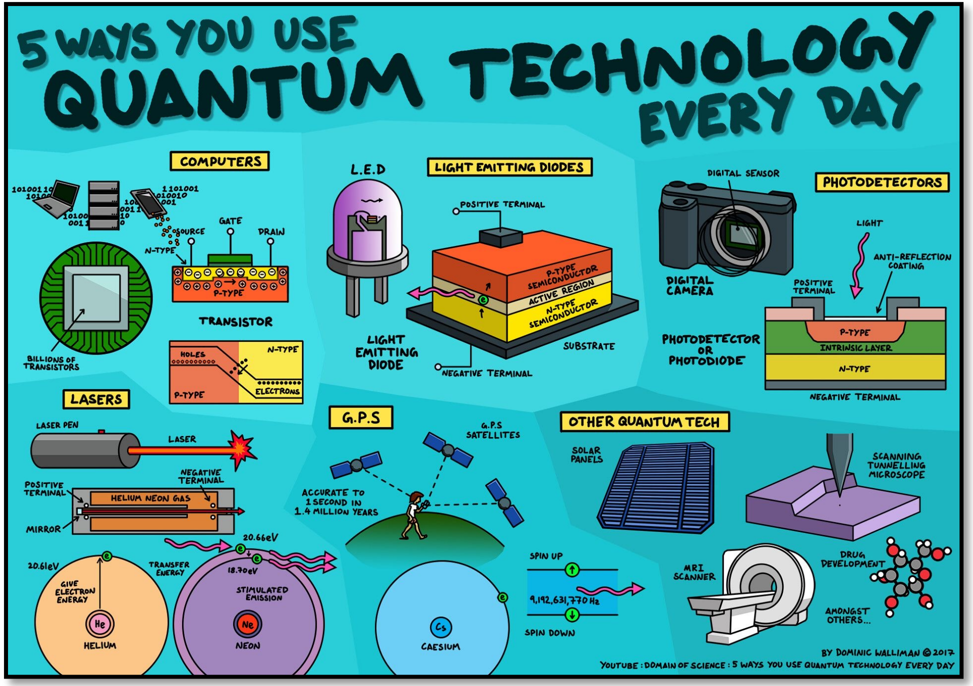
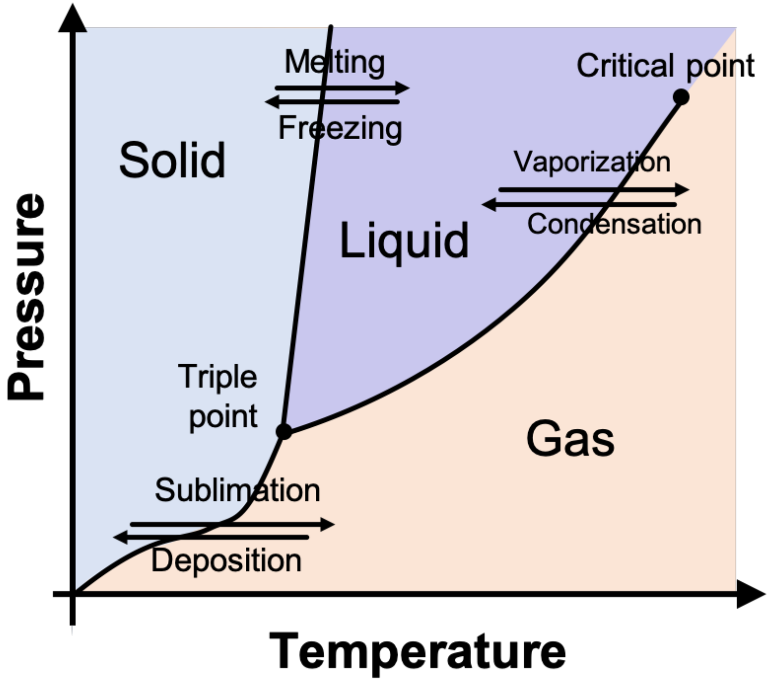


Image: Dominic Walliman

Quantum phase transitions

- Classical phase transitions can occur from thermal fluctuations
- Low-temperature behavior governed by quantum fluctuations
- Quantum fluctuations lead to surprising behavior
  - High-temperature superconductors
  - Mott Metal-Insulator transition



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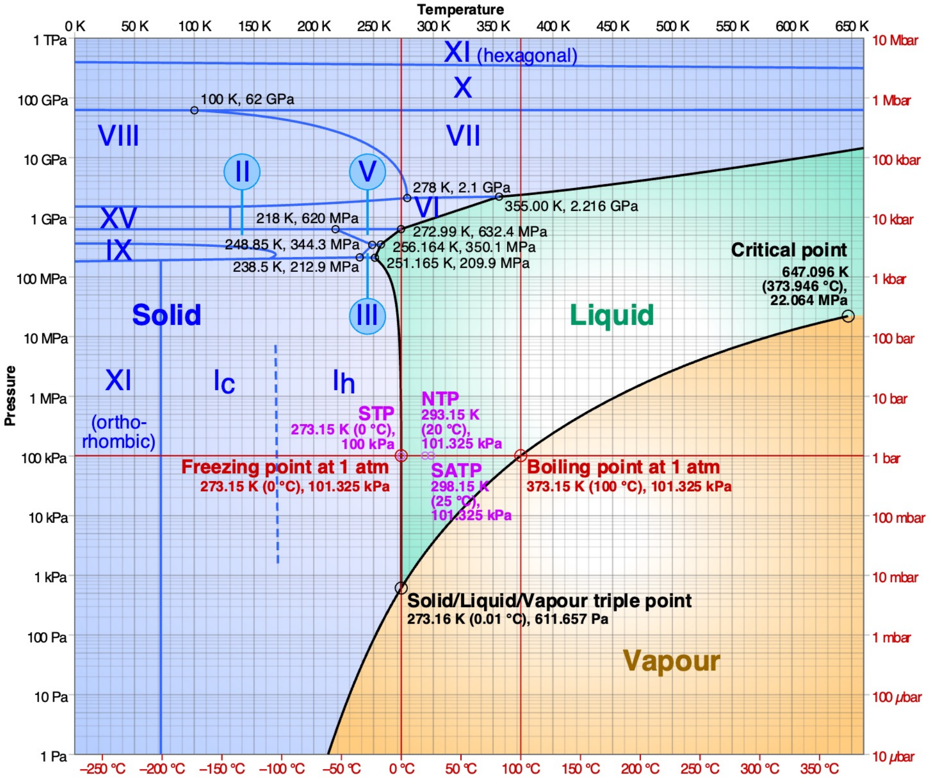

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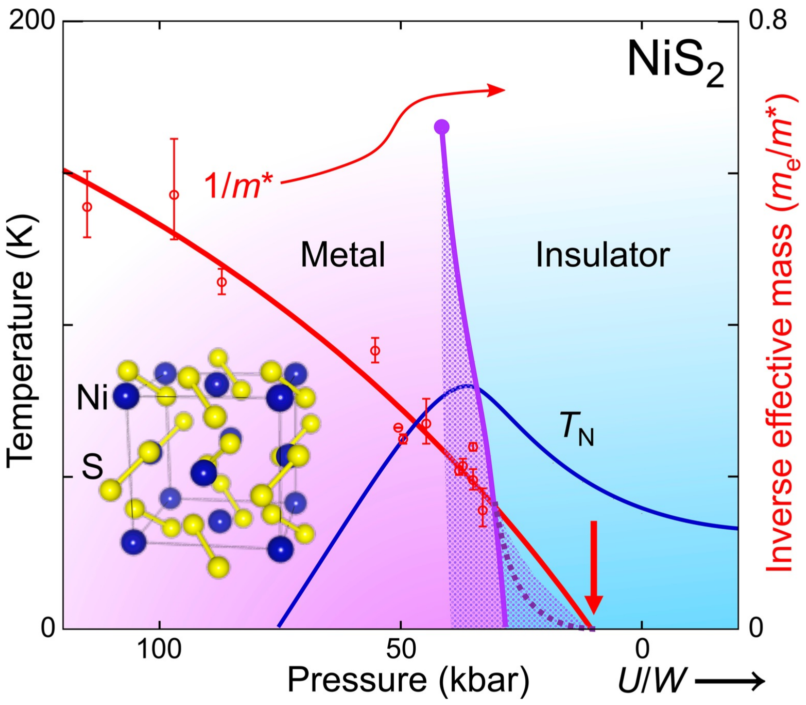

From Semeniuk et al. 10.1073/pnas.2301456120

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Interacting Many-Body Models

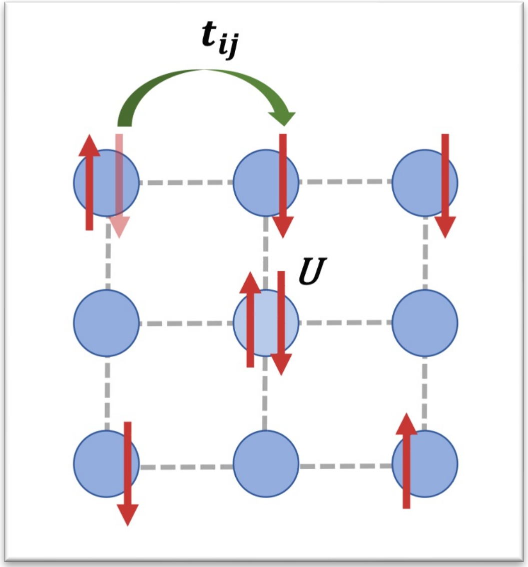
The one-band Hubbard Model

$$\hat{H}_{\text{Hubbard}} = \underbrace{\sum_{<i,j>,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + h.c.}_{\text{Kinetic energy ("hopping")}} \underbrace{- \mu \sum_{i,\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}}_{\text{Chemical potential}} \underbrace{+ U \sum_{i} \hat{c}^{\dagger}_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^{\dagger}_{i\downarrow}\hat{c}_{i\downarrow}}_{\text{Coulomb repulsion}}$$

Kinetic energy ("hopping")

Chemical potential

Coulomb repulsion



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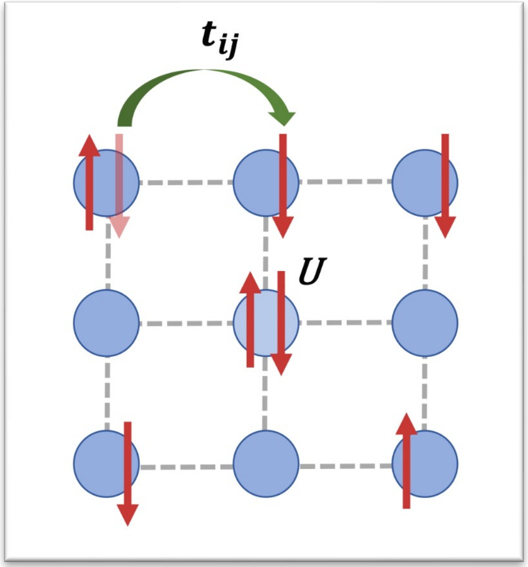


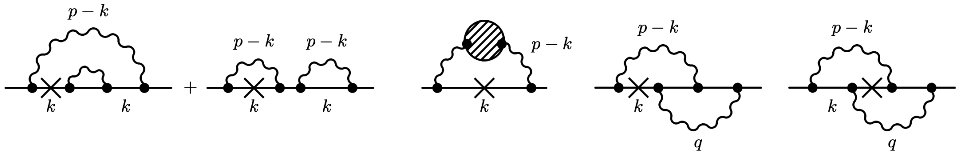
- A simple lattice model which can describe quantum phase transitions due to many-body interactions
- Strong interactions (correlations) are accounted for with the Coulomb repulsion term
  - When U is small, this model is *free-fermionic*
  - When U is large, electron-electron correlations inhibit charge transport

The one-band Hubbard Model

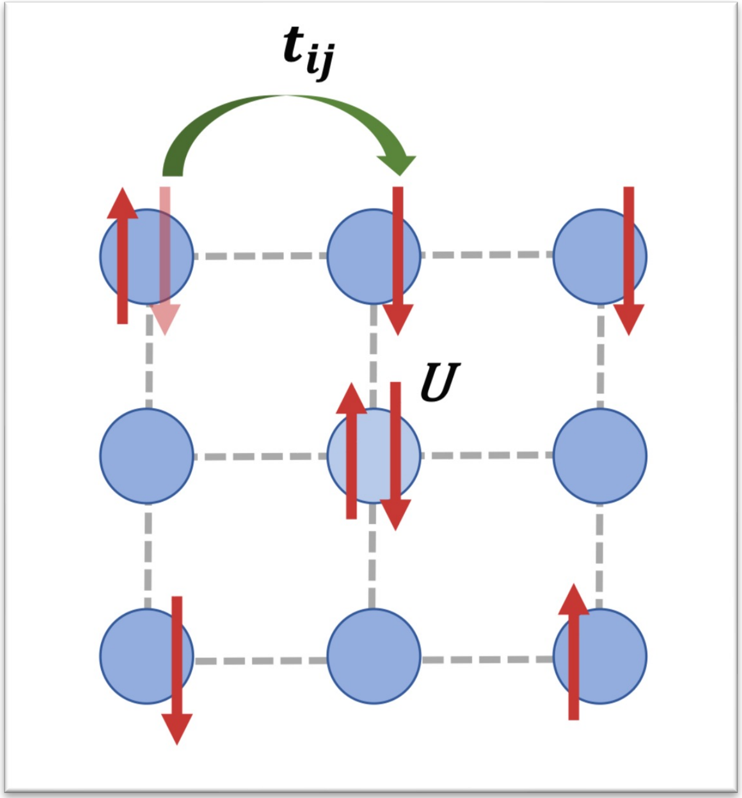
Important quantities:

$$G_{ij,\sigma}(t) = -i\langle\psi_0|\{\hat{c}_{i\sigma}(t), \hat{c}^\dagger_{j\sigma}\}|\psi_0\rangle$$

$$\Sigma_{ij,\sigma}(\omega,k) = (g^0_{ij,\sigma}(\omega,k))^{-1} - (G_{ij,\sigma}(\omega,k))^{-1}$$

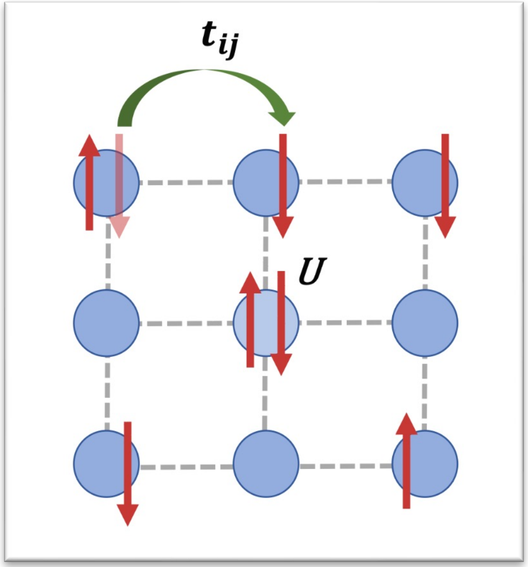


From Kotikov et al. 10.3390/particles3020026



So what's the big deal about this simple model?

The one-band Hubbard Model



- ❑ Difficult to solve classically
  - Hilbert space scales exponentially as 2^N

$$U \sum_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}$$

Coulomb repulsion

$$|100010001|011010100\rangle$$

Spin up Spin down

For 9 sites, there are 2 spins per site which require N=18 computational bits to encode

$$2^{18} \times 2^{18} = 262144 \times 262144 \approx 550\text{GB of storage}$$

$$2^{22} \times 2^{22} = 4194304 \times 4194304 \approx 140\text{TB of storage}$$

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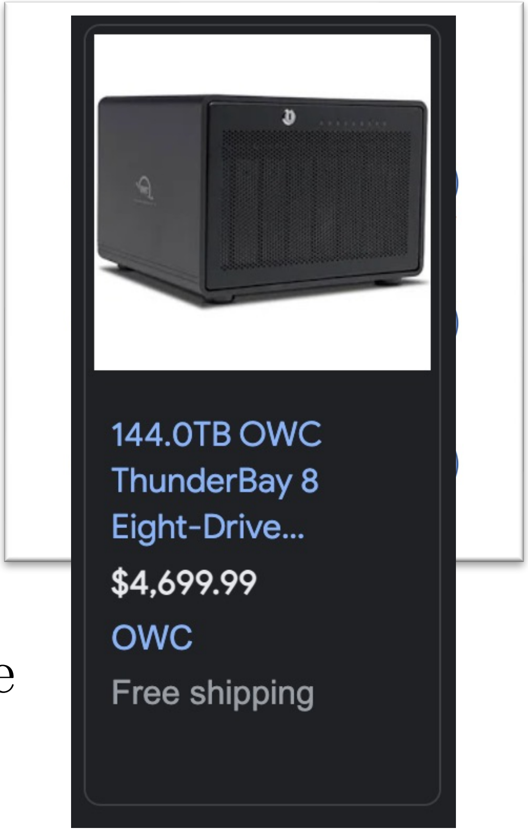
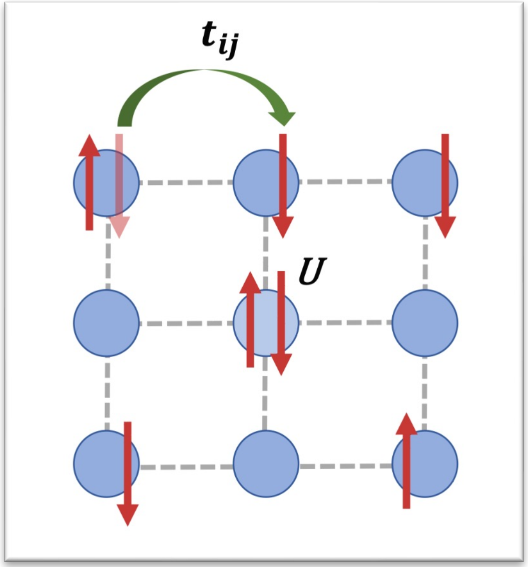


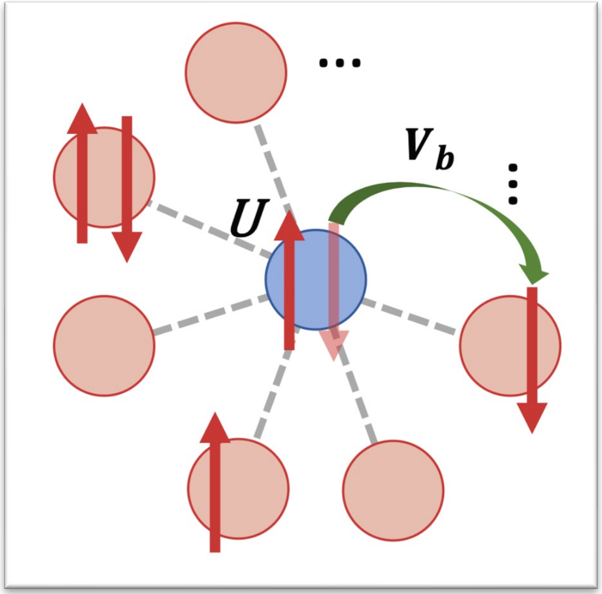
The one-band Hubbard Model

- Difficult to solve classically
  - Hilbert space scales exponentially as 2^N
- In the infinite-dimensional Hubbard model, the correlation effects become *local in space*
- Consequentially, the self-energy $\Sigma_{\text{Hubbard}}(\omega)$ is momentum-independent



$$G_{\text{Hub}}(\omega, k) = G_{\text{Hub}}(\omega) = \int d\epsilon \frac{\rho(\epsilon)}{\omega - (\epsilon - \mu) - \Sigma_{\text{Hub}}(\omega)}$$

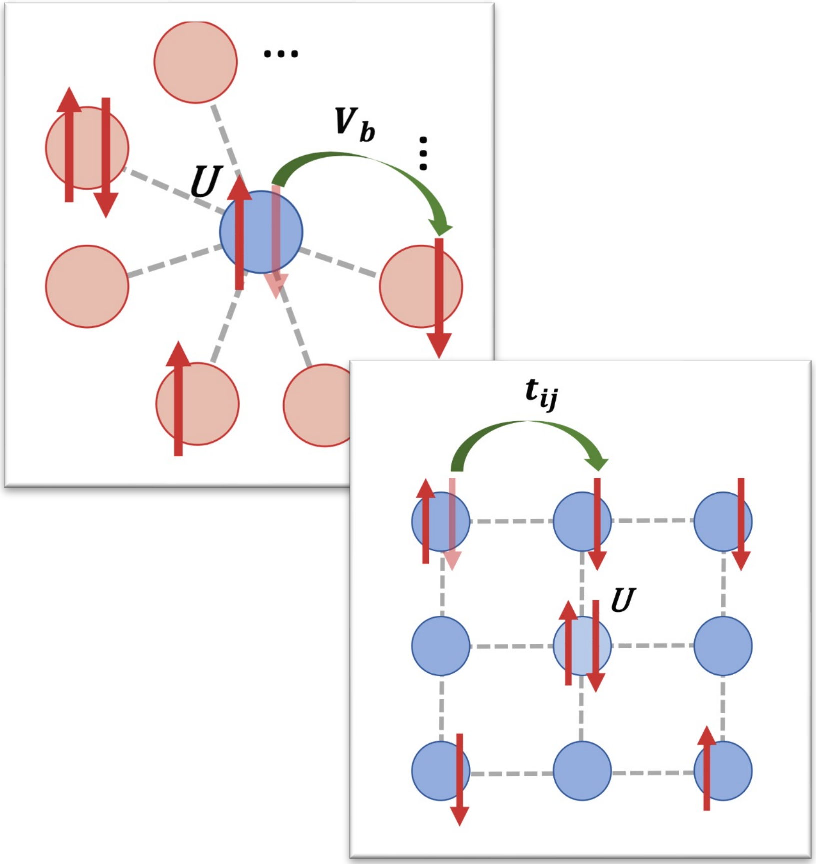
Single impurity Anderson Model (SIAM)



$$\hat{H}_{\text{impurity}} = \underbrace{\sum_{b\sigma}^{N_{\text{bath}}} V_b \hat{d}^\dagger_\sigma \hat{c}_{b\sigma} + h.c.}_{\text{Impurity-bath hopping}} + \underbrace{\sum_{b\sigma}^{N_{\text{bath}}} \epsilon_b \hat{c}^\dagger_{b\sigma} \hat{c}_{b\sigma}}_{\text{Bath on-site energy}} + \underbrace{\sum_{\sigma} (\epsilon_{\text{imp}} - \mu) \hat{d}^\dagger_\sigma \hat{d}_\sigma}_{\text{Impurity on-site energy}} + \underbrace{U \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow}_{\text{Coulomb repulsion}}$$

- Strong interactions occur *only* on the impurity site
- Electrons can only hop between a bath site and the impurity
- In the limit of infinite bath sites, this model is exactly the infinite-dimensional Hubbard model

Single impurity Anderson Model (SIAM)

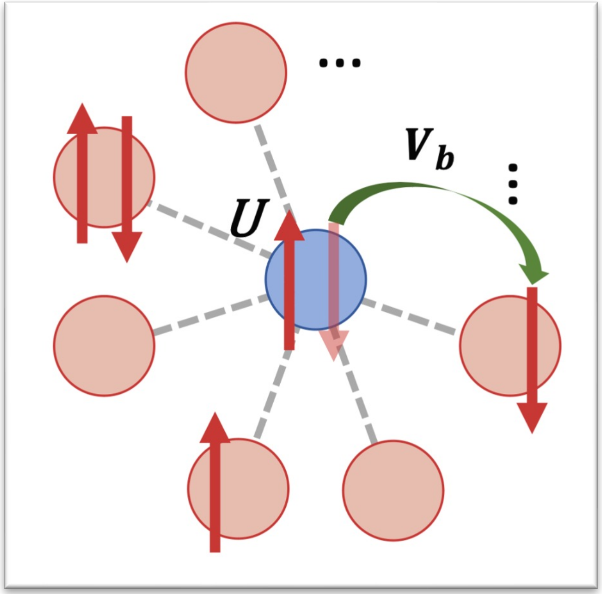


- How do we faithfully map the infinite-dimensional one-band Hubbard Model to the SIAM with a finite bath?

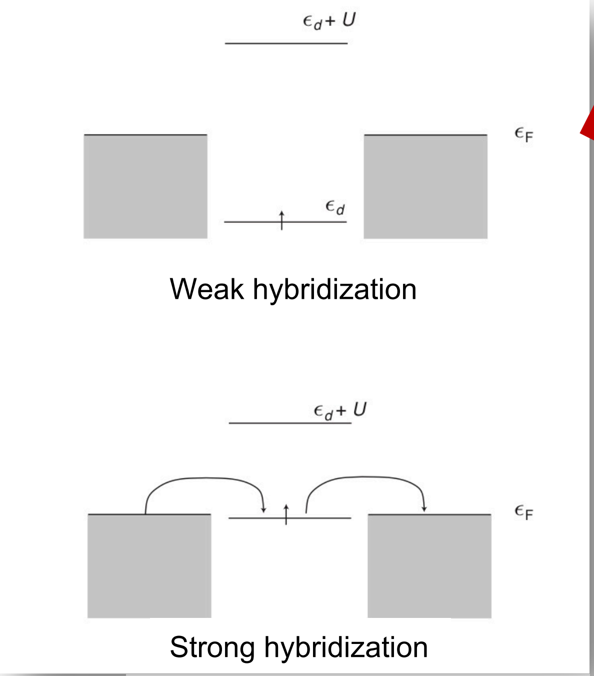
$$\Sigma_{\text{impurity}}(\omega) \approx \Sigma_{\text{Hubbard}}(\omega)$$

Both are local!

Single impurity Anderson Model (SIAM)

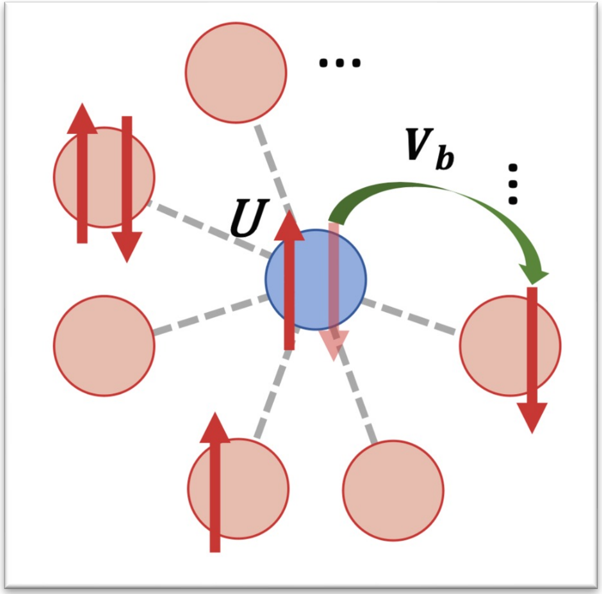


$$\mathcal{G}_{\rm imp}(\omega) = \frac{1}{\omega - (\epsilon_d - \mu) - \Delta(\omega) - \Sigma_{\rm imp}(\omega) + i\eta}$$



From Phillips, Advanced Solid State Physics

Single impurity Anderson Model (SIAM)



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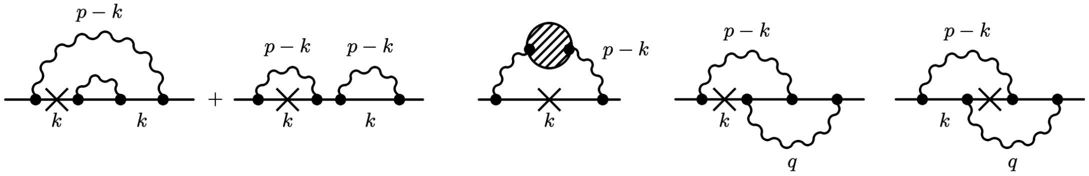

From Kotikov et al. 10.3390/particles3020026

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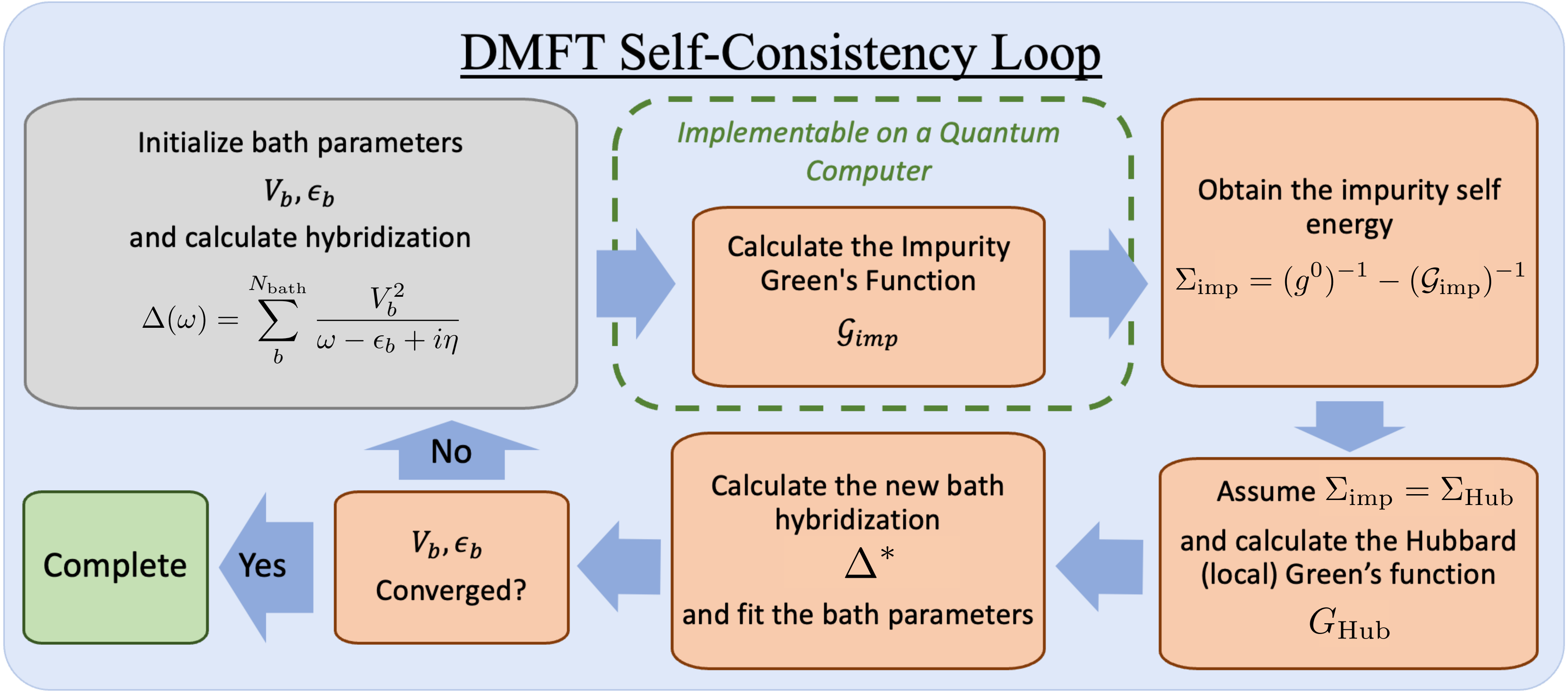
Dynamical Mean Field Theory

Self-consistency procedure



Self-consistency procedure

$$\mathcal{G}_{\text{imp}}(t) = -i\langle\psi_0|\hat{d}(t)\hat{d}^\dagger|\psi_0\rangle$$

$$\mathcal{G}_{\text{imp}}(t) = -i\langle\psi_0|e^{i\hat{H}_{\text{imp}}t}\hat{d}e^{-i\hat{H}_{\text{imp}}t}\hat{d}^\dagger|\psi_0\rangle$$

Requires saving and diagonalizing a Hilbert space of size 2^N

Self-consistency procedure

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- How can we efficiently find the ground state of the impurity model with many bath sites?
- What is the most practical way of calculating the impurity Green's function?
- What tools currently exist to assist with solving problems with exponentially scaling Hilbert spaces?

Quantum Subspace Diagonalization

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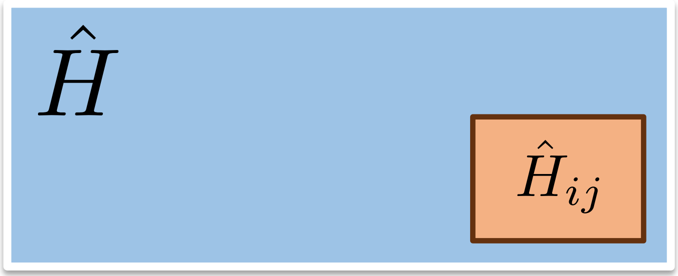
Eigenvector Continuation

- The ground state of a system is typically spanned by a few low-energy vectors
- Selecting a few low-energy vectors in parameter space can give a good approximation of the ground state



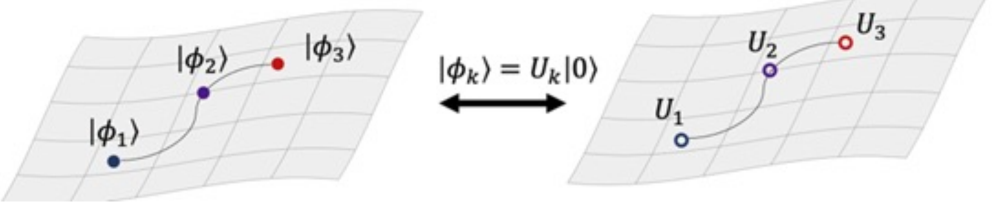
$$\hat{H}|\psi_0\rangle = \epsilon_0|\psi_0\rangle$$

$$\hat{H}_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle$$

$$S_{ij} = \langle\phi_i|\phi_j\rangle$$

$$\hat{H}_{ij}|\psi_0\rangle = \epsilon_0 S_{ij}|\psi_0\rangle$$

Parameter space



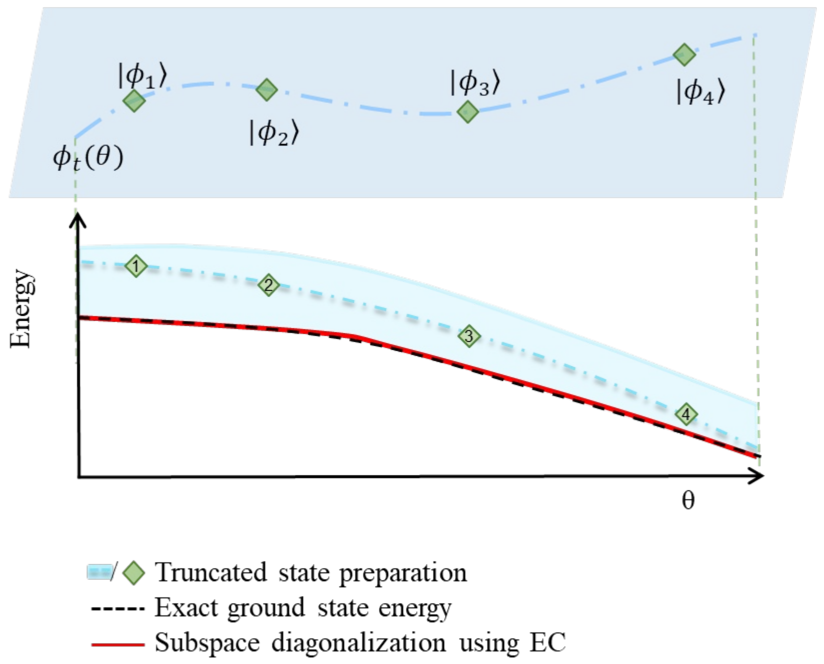
$$|\phi_3\rangle = \alpha_1|\phi_1\rangle + \alpha_1|\phi_2\rangle$$

D. Frame et.al, Phys. Rev. Lett. 121, 032501

Eigenvector Continuation

- Using Eigenvector Continuation, low-energy states can be selected in different points of parameter space and used as a subspace

- How do we find low-energy states corresponding to the impurity model?



A. Francis, et. al., 2209.10571

Mean field approximation

$$U\hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow$$

Mean-field (MF) approximation

$$\hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow \to \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \langle \hat{d}^\dagger_\downarrow \hat{d}_\downarrow \rangle + \langle \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \rangle \hat{d}^\dagger_\downarrow \hat{d}_\downarrow$$

$$\hat{H}_{\text{imp}} = \hat{H}_0 + \hat{H}_{\text{int}} \to \sum_{ij} h_{ij} \hat{c}^\dagger_i \hat{c}_j$$

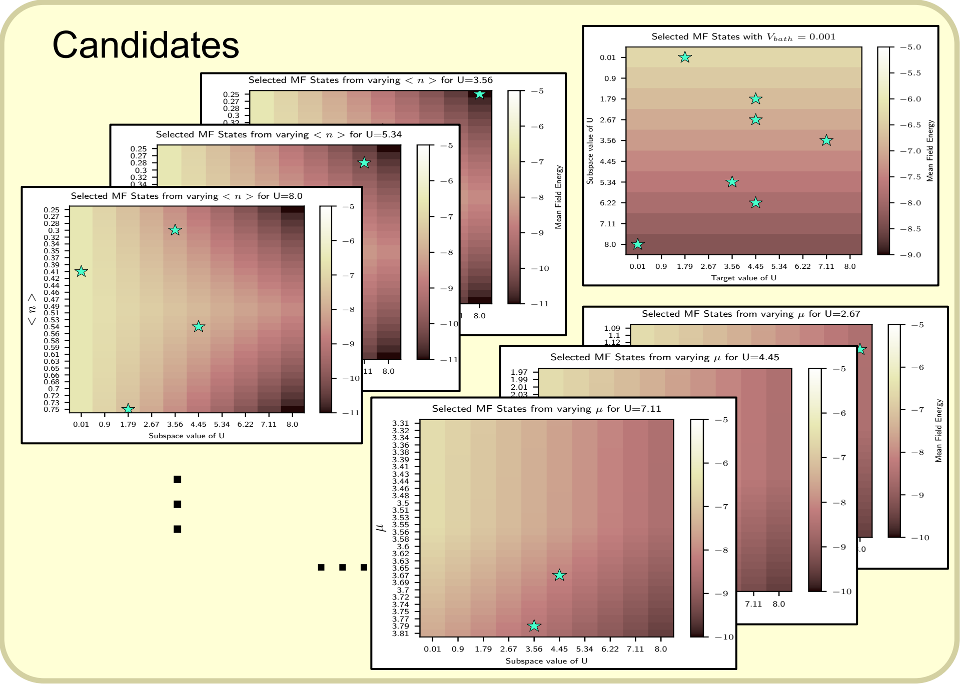
Free fermionic!

$2^N \times 2^N$ problem (for $\hat{H}_{\text{imp}}$)

$N \times N$ problem (for h_{ij})

Can ground states from this N × N mean-field problem be used as a subspace for Eigenvector Continuation?

Mean field approximation



$$\hat{H}_{\text{imp}}(\theta) \rightarrow \hat{h}_{\text{imp}}(\theta)$$

$$\theta = \{U, \epsilon_b, V_b, \mu\} \rightarrow \theta = \{(U)_i, (\epsilon_b)_i, (V_b)_i, (\mu)_i, (\langle \hat{d}^\dagger_\sigma \hat{d}_\sigma \rangle)_i\}$$

Target values

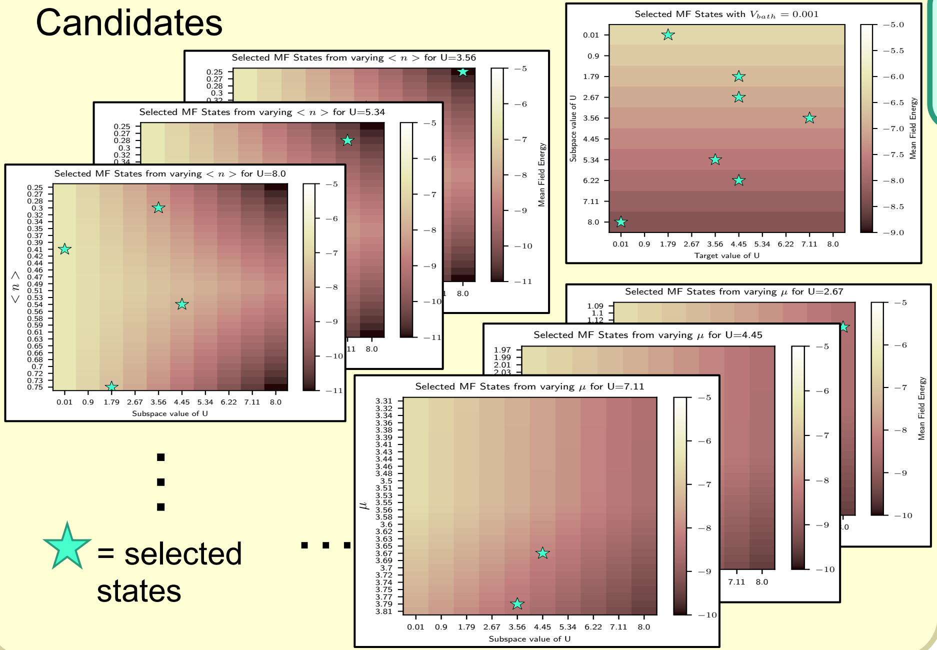
$$S_{ij} = \langle \phi_i | \phi_j \rangle$$

$$\mathbf{S}^{-1}\hat{\mathbf{H}}|\psi_0\rangle = \epsilon_0 |\psi_0\rangle$$

1. The overlap matrix must not be ill-conditioned
2. The size of the overlap matrix and smaller Hamiltonian should be less than the size of the full Hilbert space

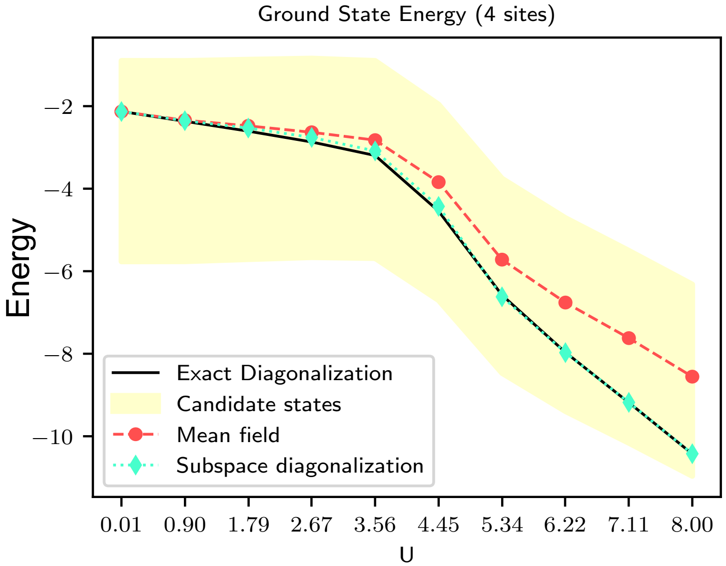
Mean field approximation

Candidates

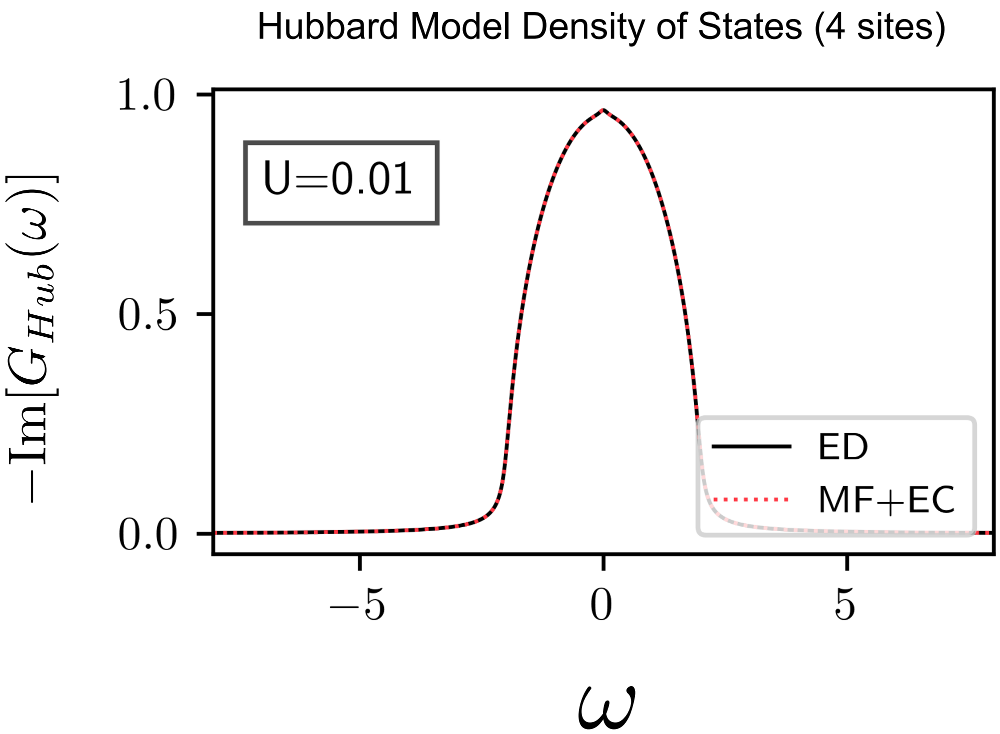


☆ = selected states

Subspace diagonalization with EC using selected states



Preliminary results



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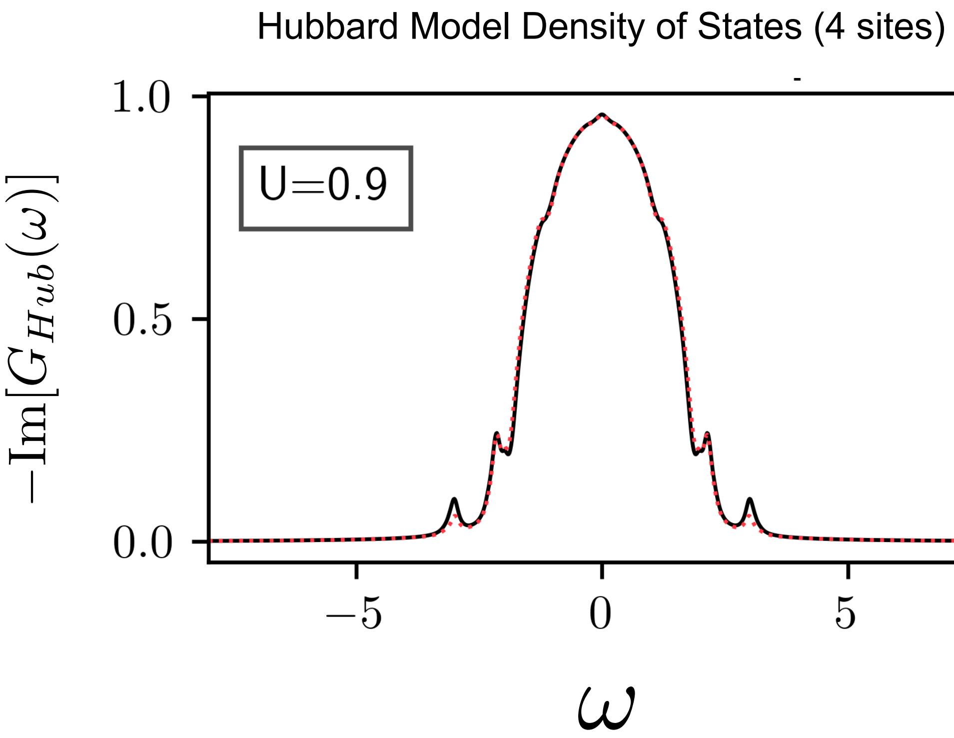

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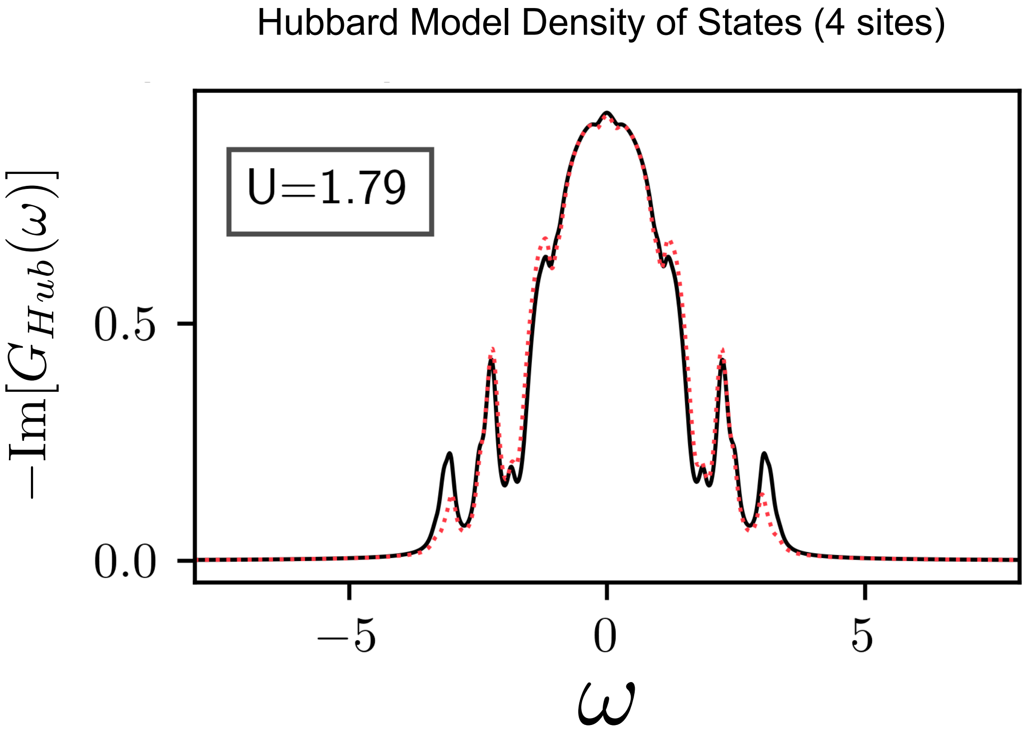

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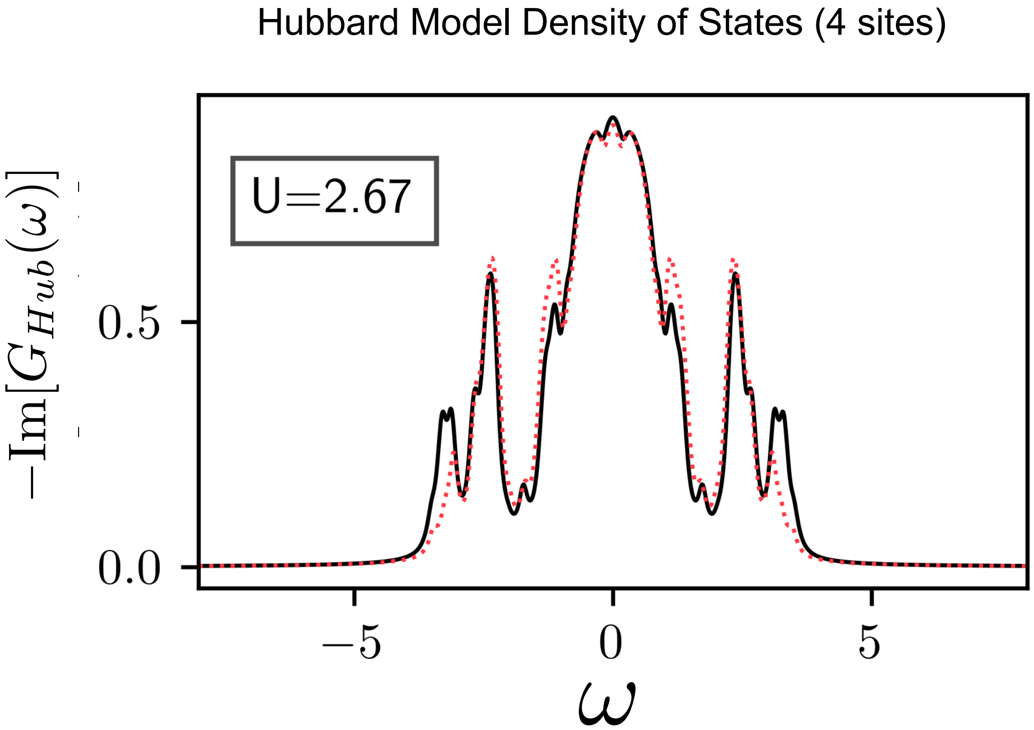

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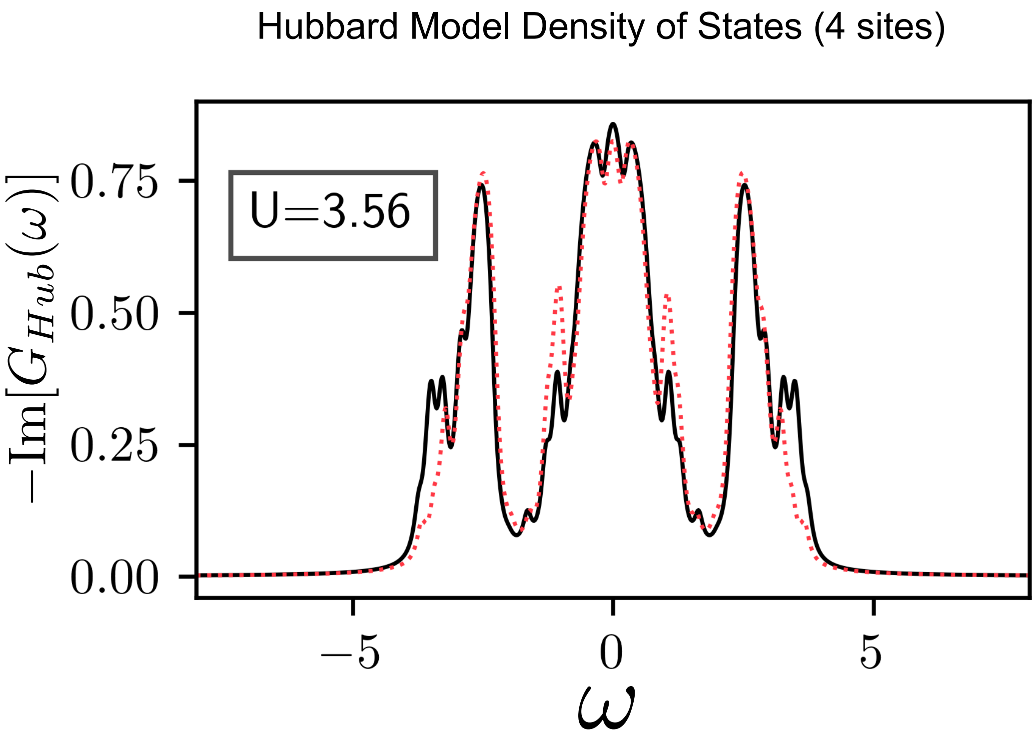

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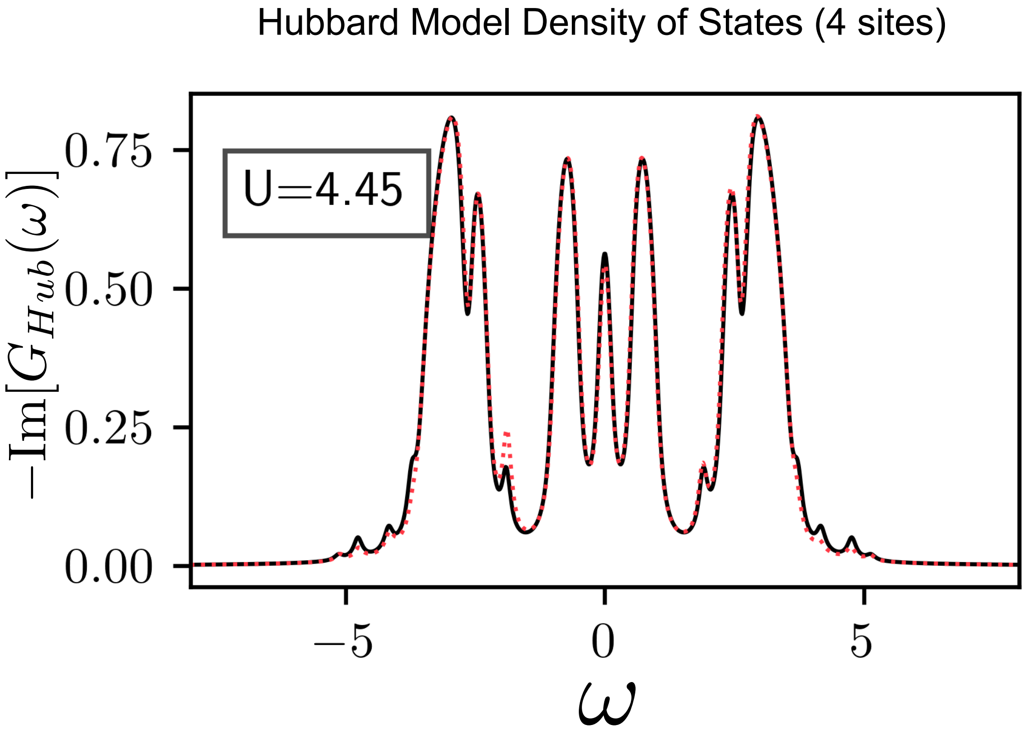

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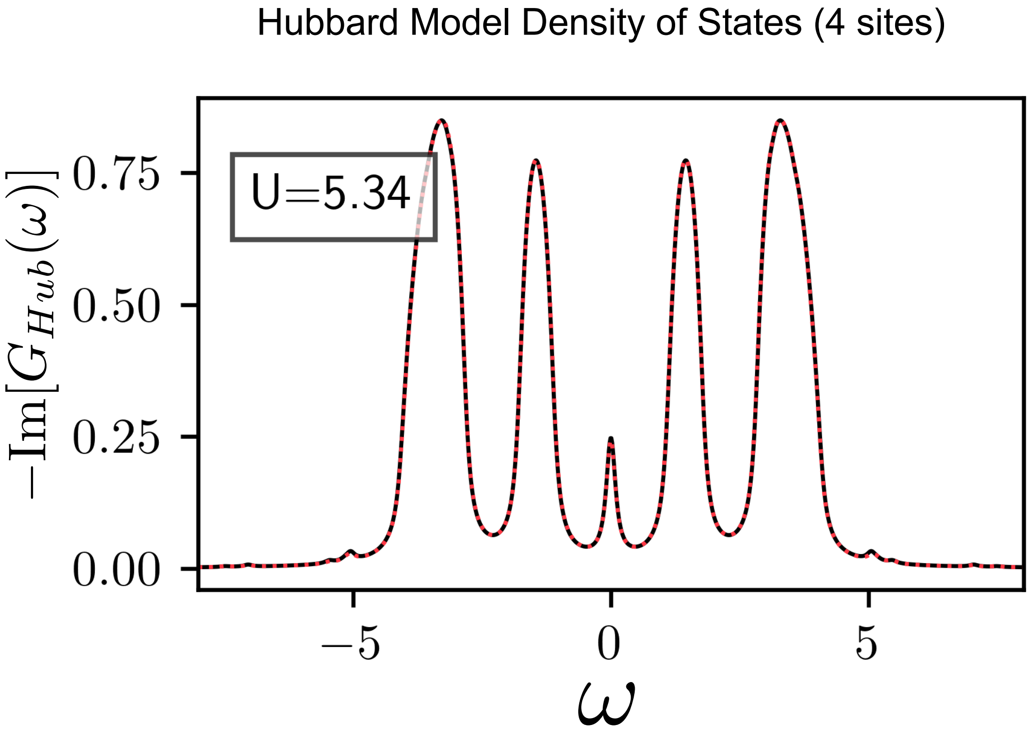

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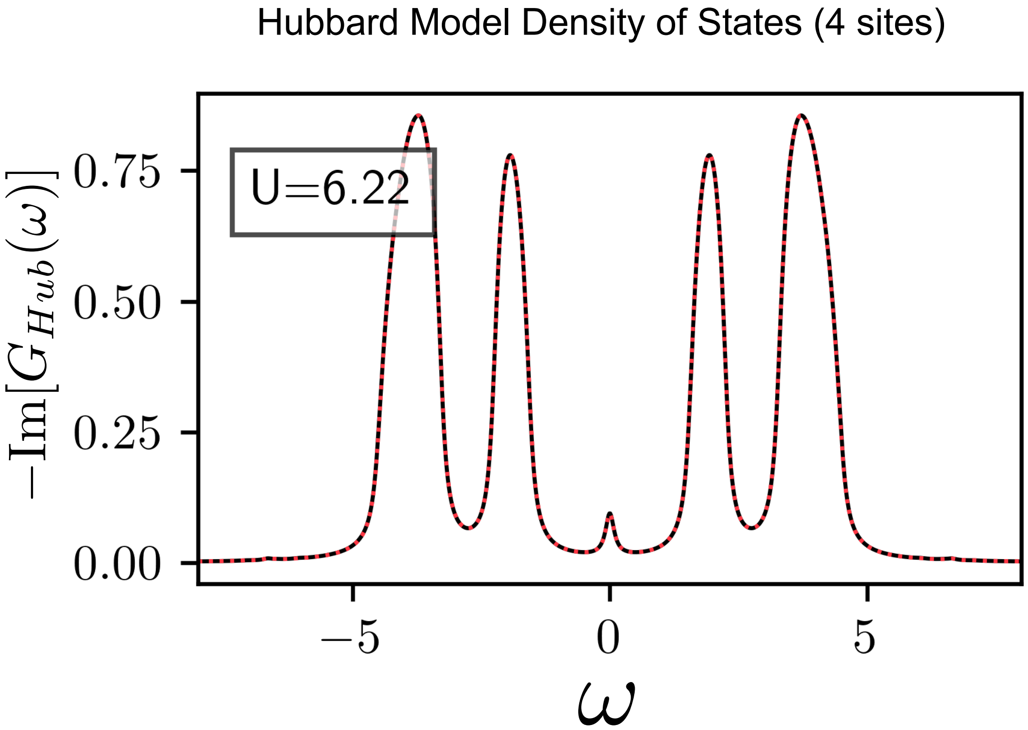

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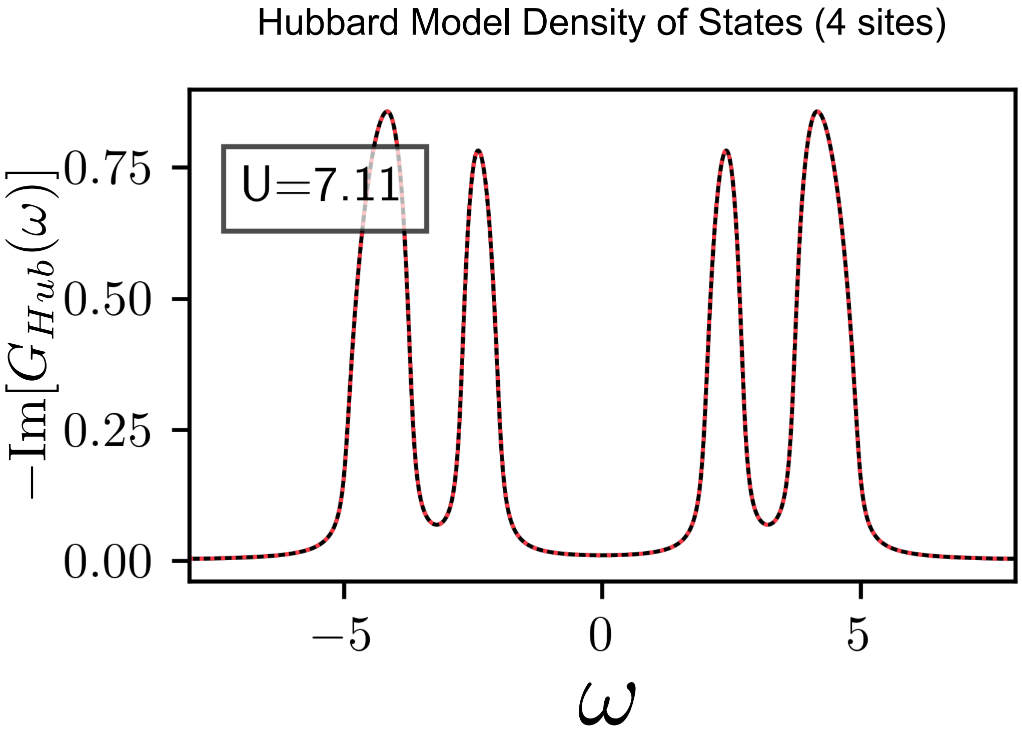

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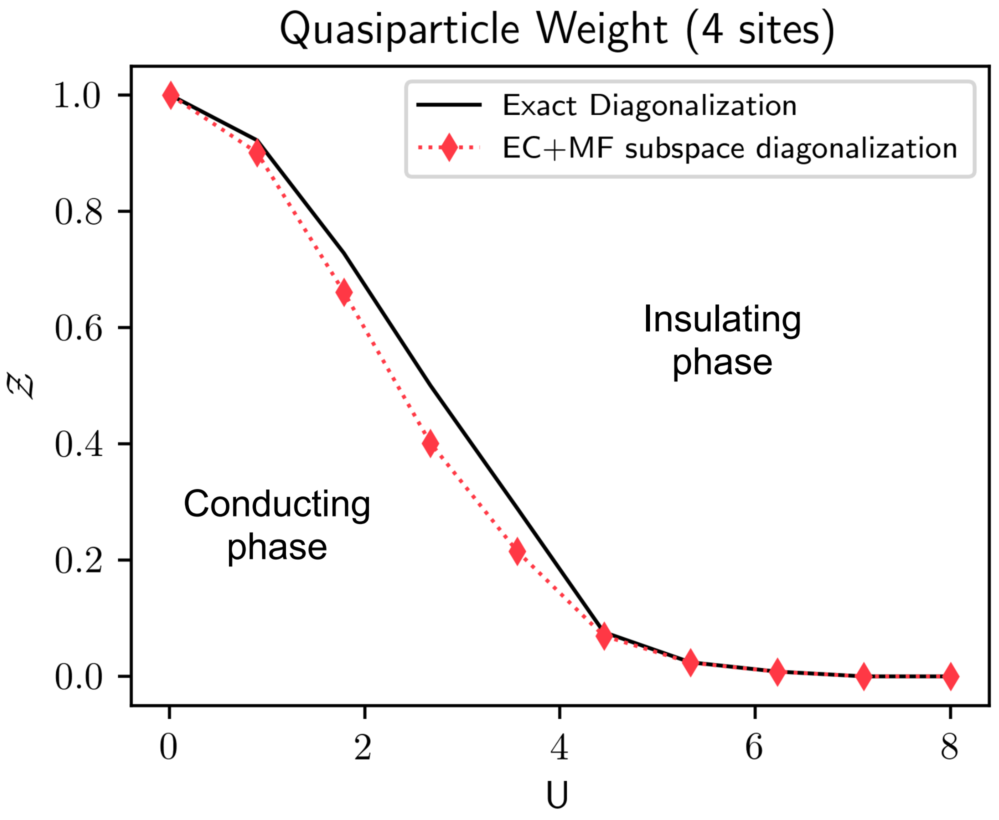
Preliminary results

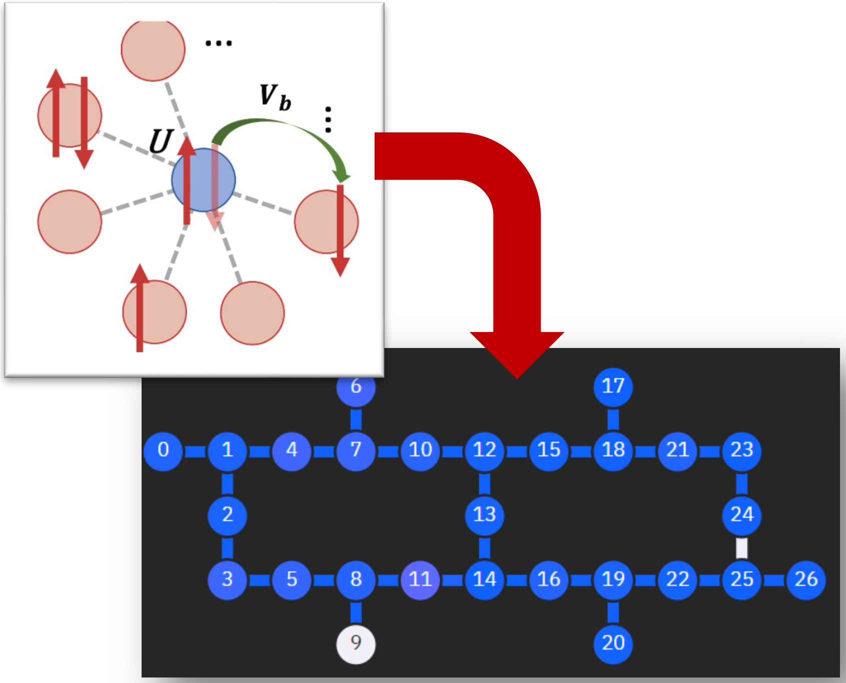
- Using Eigenvector Continuation with mean-field states, we see a metal-insulator transition!
- A maximum of 6 MF states are needed to form a reliable subspace



Quantum Computation as a Tool

Why quantum computation?

- A quantum state can be directly encoded onto qubits



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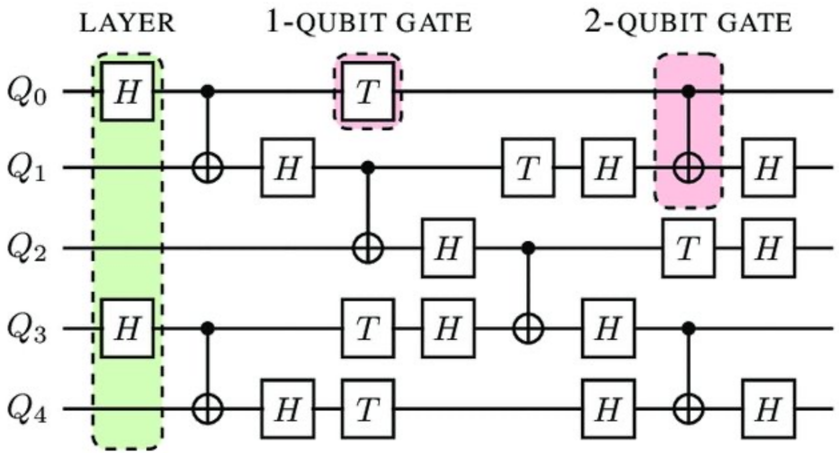
- Time evolution can be performed by unitary operations



From D. Ferrari et al. 10.1109/TQE.2021.3053921

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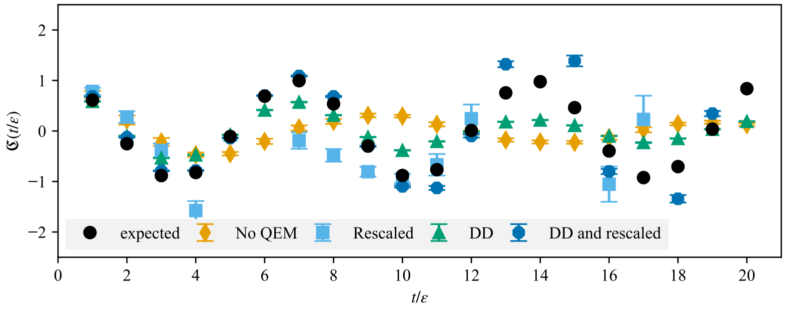
- A quantum state can be directly encoded onto qubits
- Time evolution can be performed by unitary operations
- Our system size is small enough that, with proper error mitigation and signal analysis, it is well-suited for current-term quantum devices



PHYSICAL REVIEW E **109**, 015307 (2024)

Simulating $\mathbb{Z}_2$ lattice gauge theory on a quantum computer

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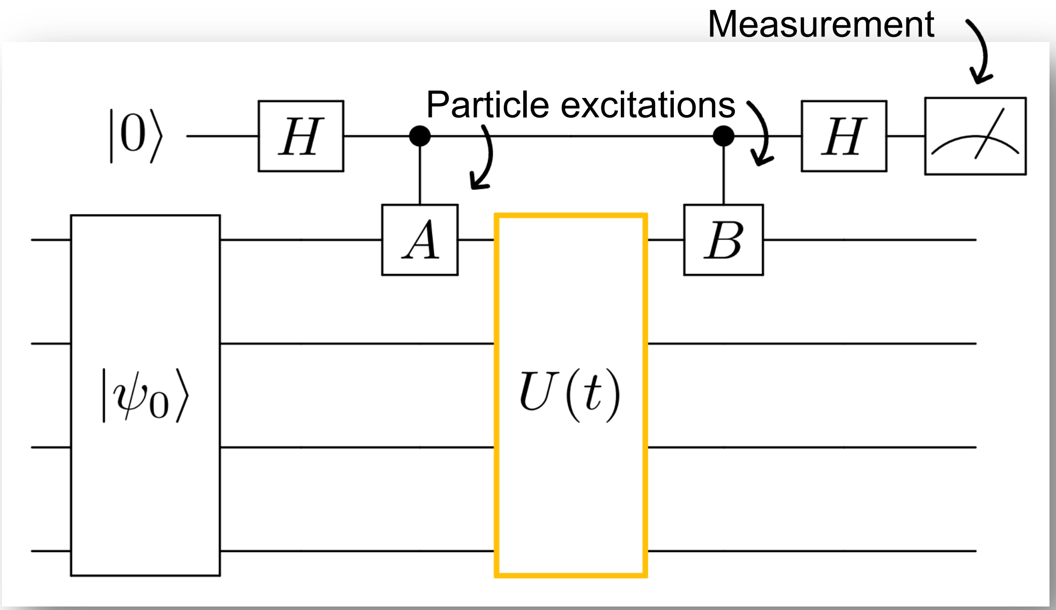
C. Charles et al. doi/10.1103/PhysRevE.109.015307

State preparation

$$\mathcal{G}_{\text{imp}}(t) =$$

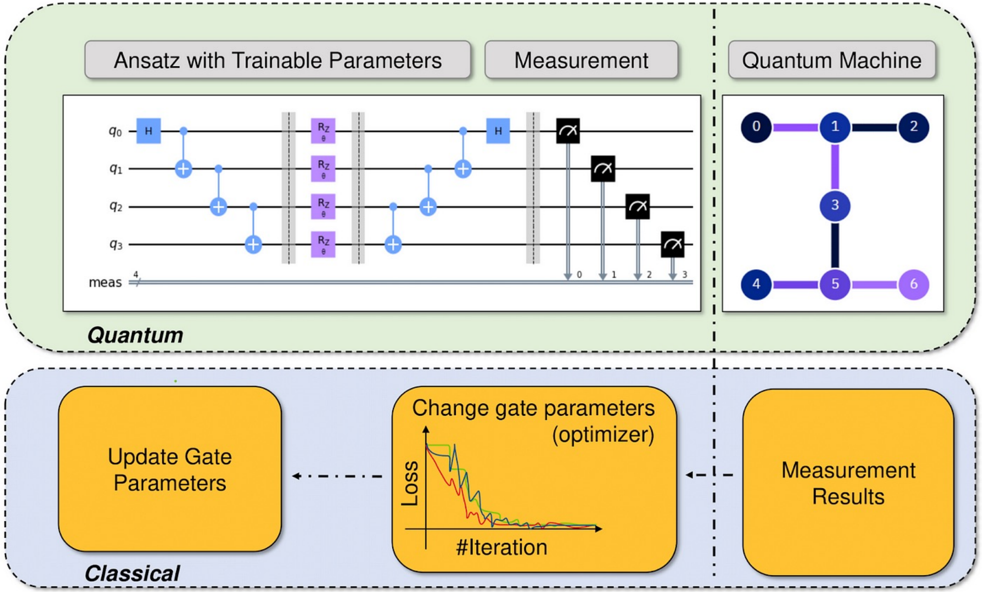


State preparation

Time evolution

State preparation

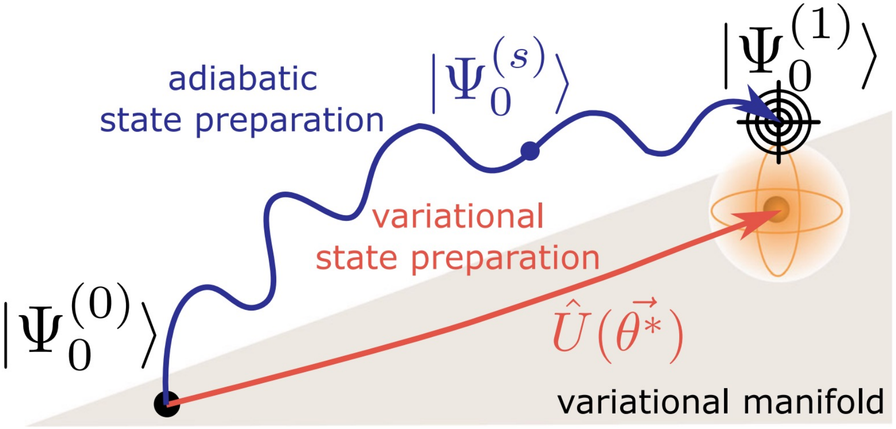
- Quantum state preparation techniques:
  - Variational methods (VQE)



From Z. Liang et al., Qiskit

State preparation

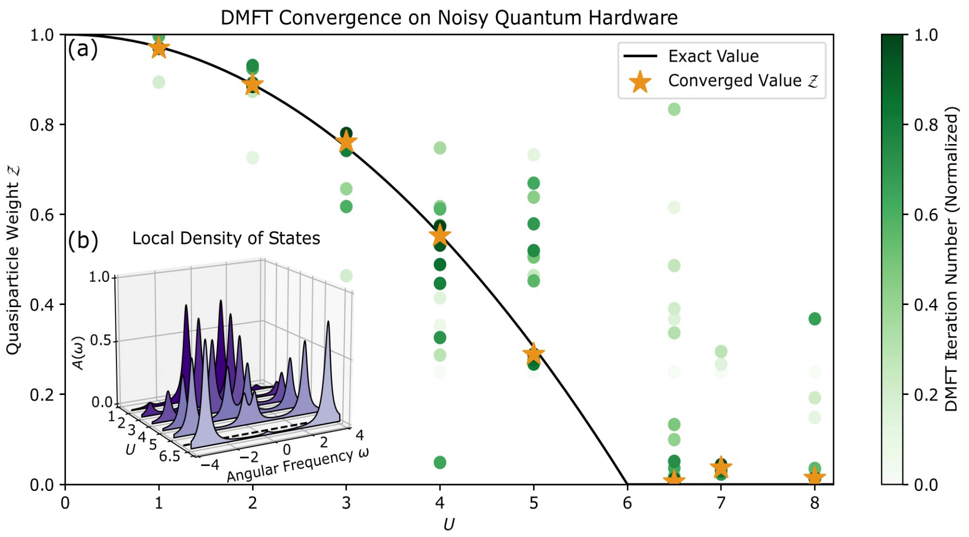
- Quantum state preparation techniques:
  - Variational methods (VQE)
  - Time evolution methods (adiabatic, imaginary)
- Being able to directly encode a free-fermionic state using a subspace of MF states will save quantum resources!



From T. Ayral et al., 10.1140/epja/s10050-023-01141-1

Time evolution

- State-of-the-art: Steckmann et al.
- Performed 2-site DMFT self-consistency on real quantum hardware
  - State prep: VQE

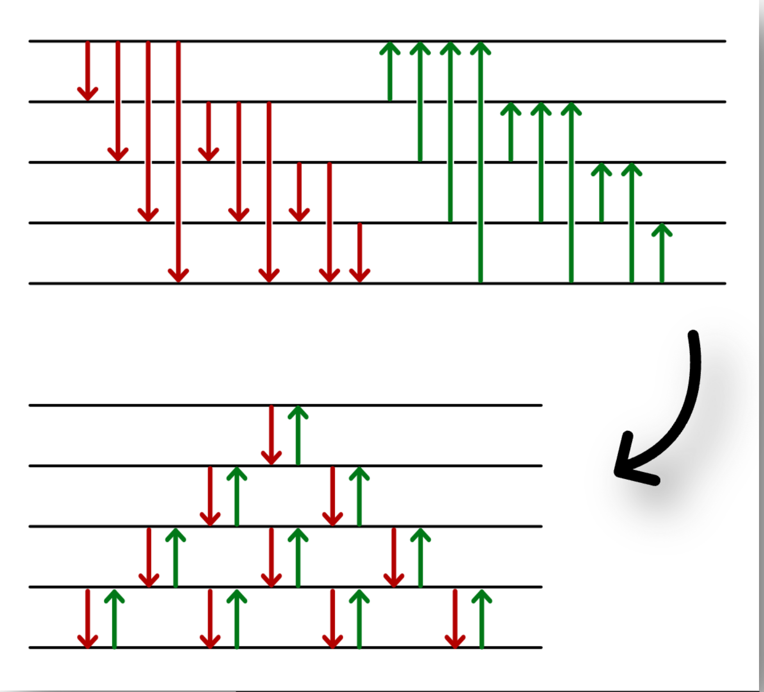


From Steckmann et al.
10.1103/PhysRevResearch.5.023198

Time evolution

- State-of-the-art: Steckmann et al.
- Performed 2-site DMFT self-consistency on real quantum hardware
  - State prep: VQE
  - Time evolution: Fast-forwarding dynamics with a fixed-depth circuit (E. Kökcü 10.1103/PhysRevLett.129.070501)

- *Future goal: Use subspace diagonalization with MF states as a state preparation technique, then use fast-forwarding circuits for time evolution on real hardware*



From E. Kökcü 10.1103/PhysRevLett.129.070501

Thank you for listening!

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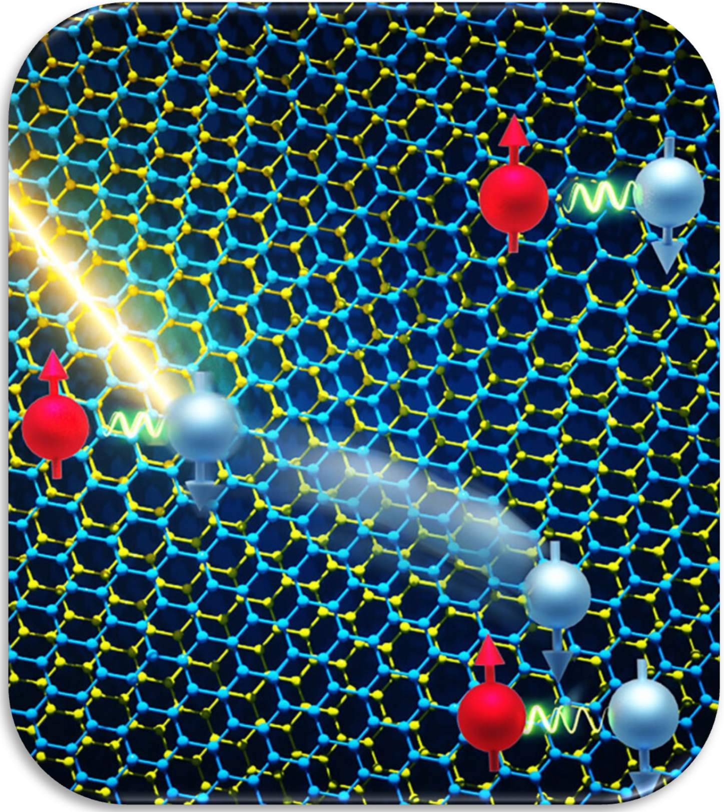
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