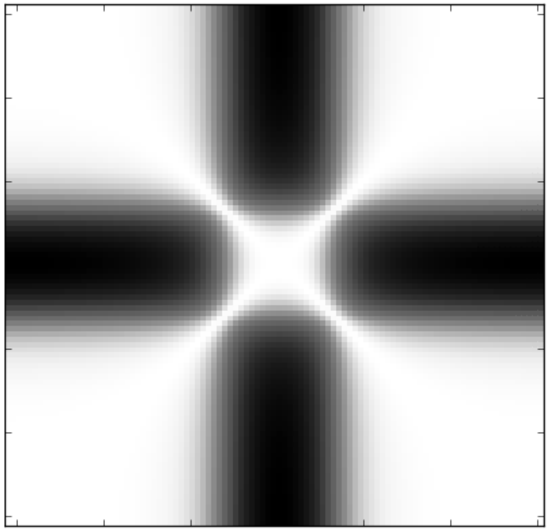
A computational approach to the inverse problem of unconventional superconductivity



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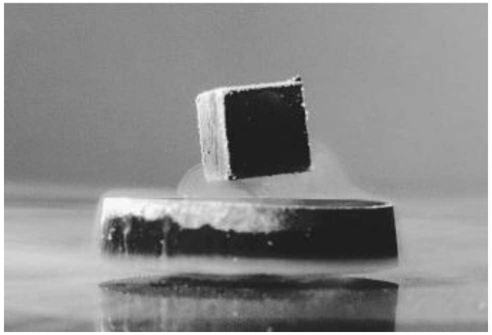
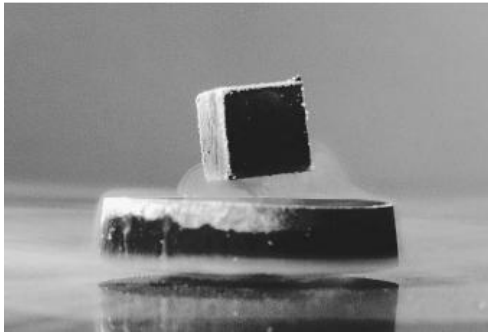
What is the inverse problem?

Forward problem: microscopic to macroscopic

$$H = -\sum_{ij,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + h.c.) - \sum_{ijkl,\sigma\tau} V_{ijkl}c^\dagger_{i\sigma}c_{j\sigma}c^\dagger_{k\tau}c_{l\tau} - \cdots$$



Inverse problem: macroscopic to microscopic

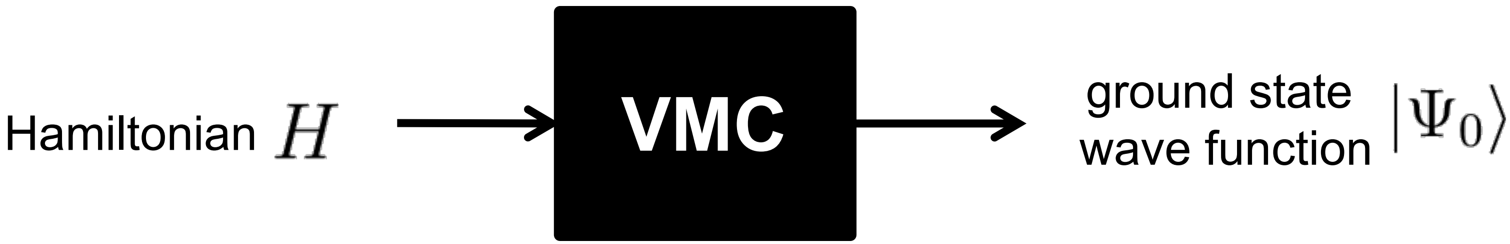


What we want to find

$$H = -\sum_{ij,\sigma} \boxed{t_{ij}}(c^\dagger_{i\sigma}c_{j\sigma} + h.c.) - \sum_{ijkl,\sigma\tau} \boxed{V_{ijkl}}c^\dagger_{i\sigma}c_{j\sigma}c^\dagger_{k\tau}c_{l\tau} - \cdots$$

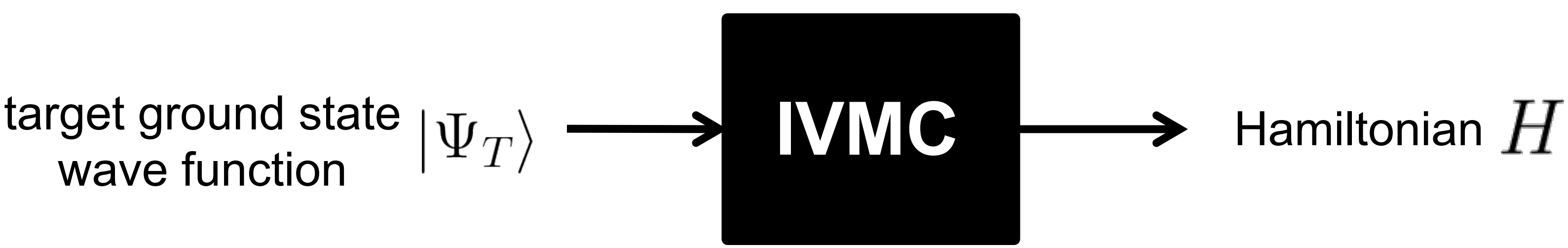
Variational and Inverse Variational Monte Carlo (VMC and IVMC)

Forward problem:



Objective: Minimize the energy $\langle H \rangle$

Inverse problem:



Objective: Minimize the energy variance σ_H^2

Minimizing the energy variance

The objective function to minimize is

$$\sigma_H^2 = \langle \Psi_T | H^2 | \Psi_T \rangle - \langle \Psi_T | H | \Psi_T \rangle^2$$

Suppose that

$$\hat{H} = \sum_a g_a \hat{h}_a$$

For example, $g_1, g_2 = t, U$ for the Hubbard model.

Then, the variance can be written as the quadratic equation

$$\sigma_H^2 = \mathbf{g}^T \mathbf{S} \mathbf{g} \qquad S_{ab} = \langle \hat{h}_a \hat{h}_b \rangle - \langle \hat{h}_a \rangle \langle \hat{h}_b \rangle$$

Minimizing the variance can be stated as an **eigenvalue problem**

$$\boxed{\mathbf{S}\mathbf{g}_0 = \sigma_0^2 \mathbf{g}_0} \quad \Leftrightarrow \quad \mathbf{g}_0 = \mathrm{argmin}_{\mathbf{g}} \sigma_H^2$$

$$(\mathbf{g} \text{ normalized})$$

Steps of IVMC

1. **Sample $|\Psi_T\rangle$ using Markov Chain MC to compute the matrix**

$$S_{ab} = \langle \hat{h}_a \hat{h}_b \rangle - \langle \hat{h}_a \rangle \langle \hat{h}_b \rangle$$

2. **Diagonalize**

$$\mathbf{S} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1}$$

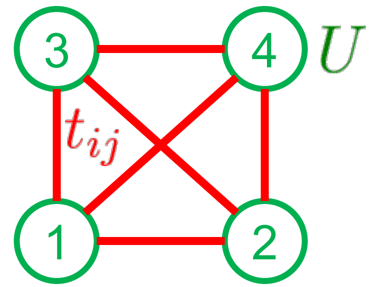
3. **Find the eigenvector(s) with the smallest eigenvalue**

$$\mathbf{S}\mathbf{g}_0 = \sigma_0^2 \mathbf{g}_0 \qquad \mathbf{g}_0 = \text{solution}$$

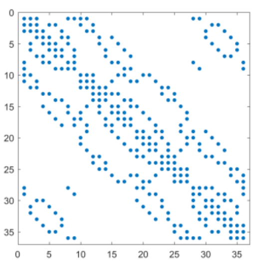
Proof of principle test

2x2 square lattice Hubbard model at half-filling

$$H = -\sum_{ij,\sigma} t_{ij}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



$t_{12} = 0.115,\quad t_{13} = -0.461, t_{14} = -0.137,$
$t_{23} = 0.0689, t_{24} = 0.358,\quad t_{34} = 0.350$ $\quad U = 0.707$

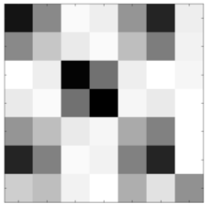


Find ground state using ED

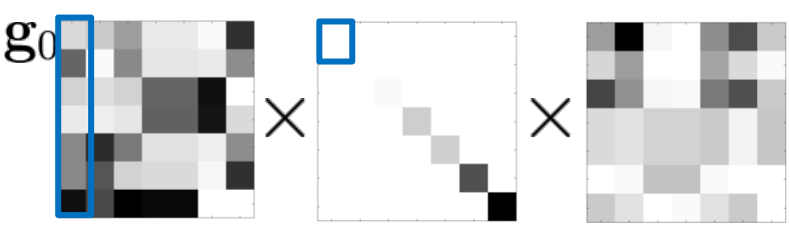
$|\Psi_0\rangle$

Find Hamiltonian using IVMC

$\mathbf{S} =$



$\mathbf{S} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1} =$



$$\mathbf{g}_0^T = (0.115, -0.461, -0.137, 0.0689, 0.358, 0.350, 0.707)$$

Searching for superconducting ground states

Superconducting target wave function

Gutzwiller-projected BCS wave function

$$
\begin{aligned}
|\Psi_T\rangle &= P_N P_g |BCS\rangle \\
&= P_N \prod_i \left(1-(1-g)n_{i\uparrow}n_{i\downarrow}\right) \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|0\rangle
\end{aligned}
$$

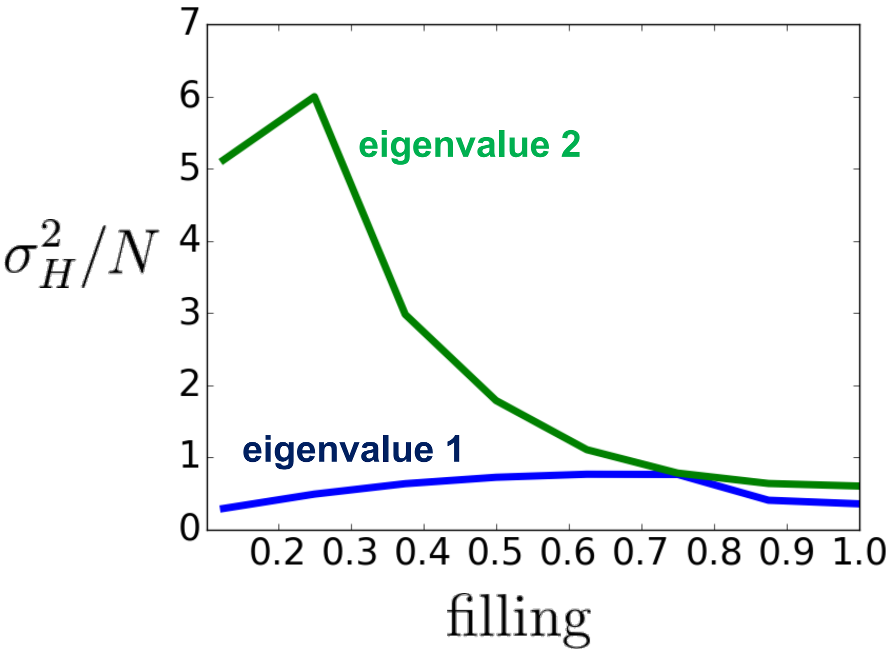
with d-wave order.

2D inhomogenous Hubbard Hamiltonians

$$
H = -t \sum_{\langle ij\rangle \sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + h.c.\right) - t' \sum_{\langle\langle ij\rangle\rangle \sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + h.c.\right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \qquad \mathbf{g} = \begin{pmatrix} -t \\ -t' \\ U \end{pmatrix}
$$

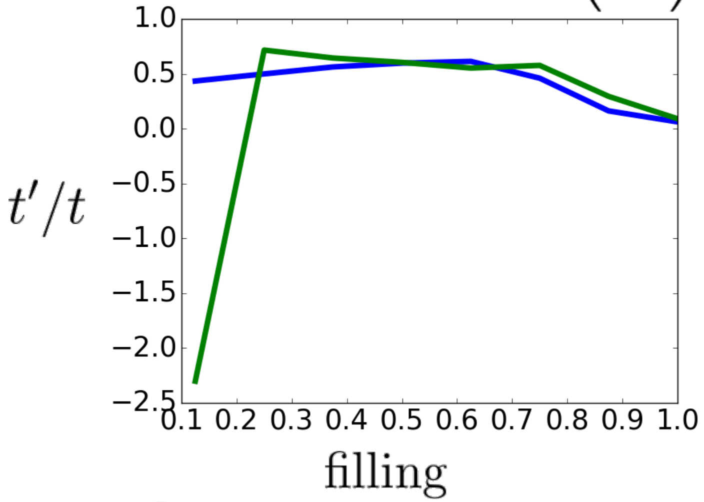
Preliminary results for projected BCS states

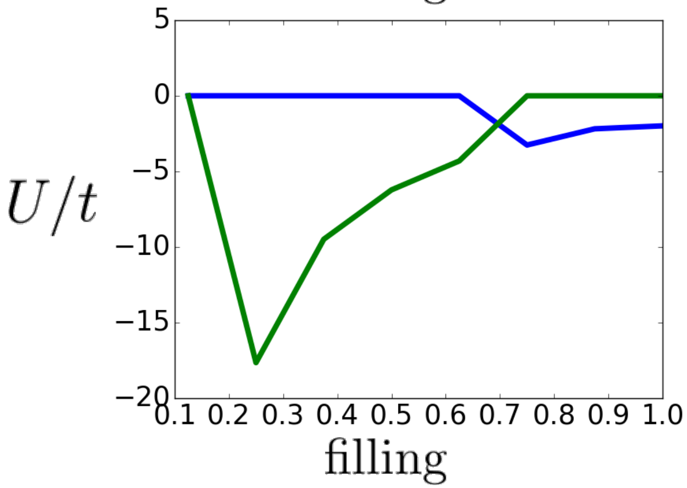
Eigenvalues of $S_{ab} = \langle h_a h_b \rangle - \langle h_a \rangle \langle h_b \rangle$



$$|\Psi_T\rangle = P_N P_g |BCS\rangle$$

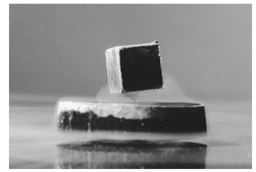
Eigenvectors $\mathbf{g} = \begin{pmatrix} -t \\ -t' \\ U \end{pmatrix}$





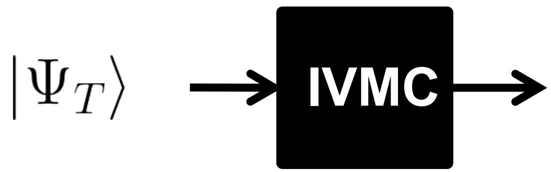
Summary

Inverse problem

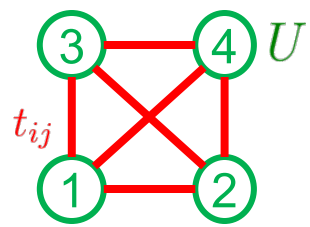


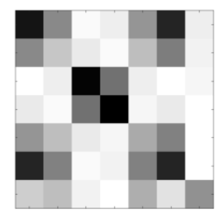
$\rightarrow$ H

IVMC



Test of IVMC





Preliminary results on superconductivity