# Useful similarity transformations for the two-dimensional repulsive Hubbard model

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## Introduction and Goals

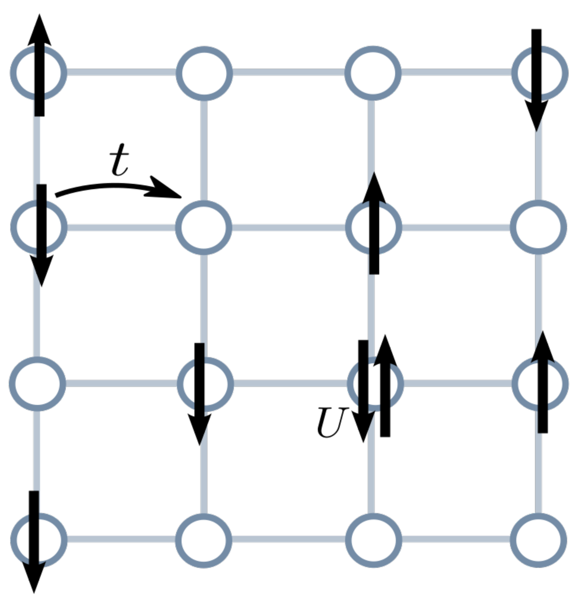
Similarity transformation of the Hubbard Hamiltonian using a **Gutzwiller correlator** leads to a *non-Hermitian* effective Hamiltonian[1,2], which can be expressed exactly in momentum-space representation and contains *three-body* interactions. While using the **kinetic** term as the **correlator** leads to *two-body* interactions in the real-space representation. We apply this methodology to study the two-dimensional Hubbard model with repulsive interactions near half-filling in the intermediate interaction strength regime ($U/t = 4$). We show that at optimal or near optimal strength of the Gutzwiller correlator, the similarity transformed Hamiltonian has extremely **compact right eigenvectors**, which can be sampled to *high accuracy* using the Full Configuration Interaction Quantum Monte Carlo (FCIQMC) method[3]. *Near-optimal correlators* can be obtained using a simple *projective* equation[2], thus obviating the need for a numerical optimisation of the correlator. Results are provided in lattice sizes upto 50 sites and compared to auxillary-field QMC[4,5].

## The Similarity Transformed Hubbard Model

**Hubbard model:** Important basic model in solid state physics

Describes a tight-binding model including local Coulomb interaction

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$




- Analytic solution exists only in one and infinite dimension
- Captures Mott insulating behaviour, antiferromagnetism and superconductivity
- Application in high-$T_C$ superconductivity

**Similarity Transformation (ST):**

- *Jastrow*-like Ansatz for the GS the wave function: $|\Psi\rangle = e^{\hat{\tau}} |\Phi\rangle$
  - *Gutzwiller* on-site correlator $\hat{\tau} = J \sum_i n_{i\uparrow} n_{i\downarrow}$ for small $U$ in k-space
  - *Neighbor-hopping* correlator $\hat{\tau} = J' \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma}$ for large $U$ in real-space
- Solve $\bar{H} |\Phi\rangle = E |\Phi\rangle$ with the Gutzwiller ST non-Hermitian H in *k-space*:

$$e^{-\tau} \hat{H} e^{\tau} = -t \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) n_{\mathbf{k},\sigma} + \frac{1}{M} \sum_{\mathbf{pqk}\sigma} \omega_2(J, \mathbf{p}, \mathbf{k}) c_{\mathbf{p}-\mathbf{k},\sigma}^\dagger c_{\mathbf{q}+\mathbf{k},\bar{\sigma}}^\dagger c_{\mathbf{q},\bar{\sigma}} c_{\mathbf{p},\sigma}$$
$$+ \frac{t(\cosh J - 1)}{M^2} \sum_{\mathbf{pqskk}'\sigma} \epsilon(\mathbf{p} - \mathbf{k} + \mathbf{k}') c_{\mathbf{p}-\mathbf{k},\sigma}^\dagger c_{\mathbf{q}+\mathbf{k}',\bar{\sigma}}^\dagger c_{\mathbf{s}+\mathbf{k}-\mathbf{k}',\bar{\sigma}}^\dagger c_{\mathbf{s},\bar{\sigma}} c_{\mathbf{q},\bar{\sigma}} c_{\mathbf{p},\sigma}$$

and the hopping ST in *real-space*:

$$\bar{H} = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l}} F(J', \mathbf{i}, \mathbf{j}, \mathbf{k}, \mathbf{l})\, c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{j}\downarrow}^\dagger c_{\mathbf{k}\downarrow} c_{\mathbf{l}\uparrow}$$

## Analytic results for the Hubbard Model

**Optimize J** by a projection of the eigenvalue equation $(\bar{H} - E)|\Phi_0\rangle = 0$ of a single reference determinant on the basis of the correlation factor:

$$\langle (\hat{\tau} - \langle \hat{\tau} \rangle)^\dagger \bar{H} \rangle = \langle \hat{\tau}^\dagger \bar{H} \rangle_c = 0$$

- For an *infinite* system at *half-filling* and *small* $U/t$ and *neglecting* the 3-body term, we obtain an optimal J: $J = \sinh^{-1}\left(\frac{5U\pi^6}{288t(16+\pi^4)}\right)$
- The energy per site can be estimated as: $E_J = -\frac{16t}{\pi^2} + \frac{U}{4} - \frac{4tJ^2}{\pi^6}(\pi^4 + 16)$

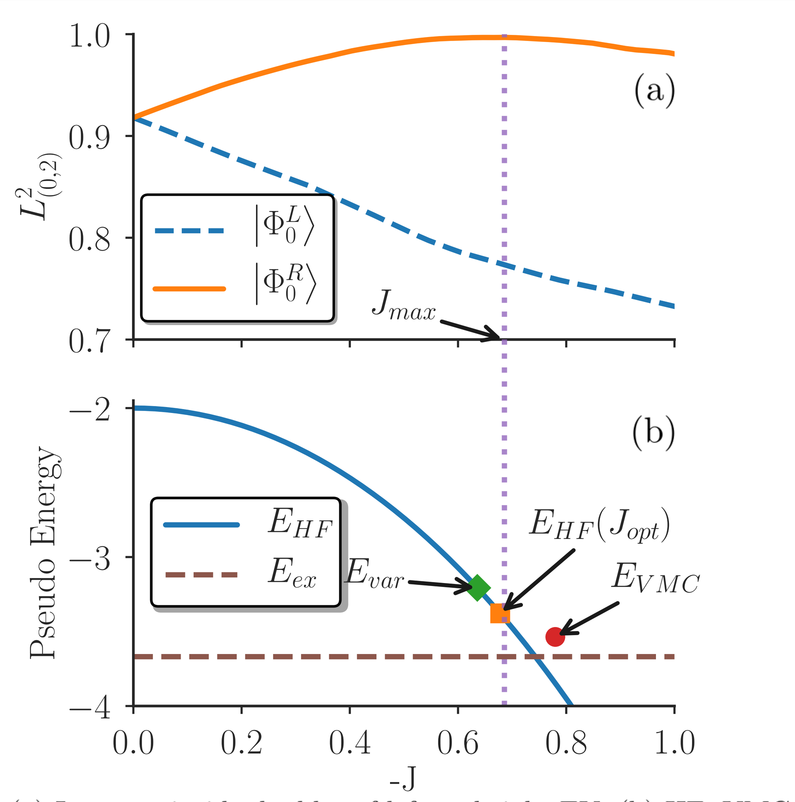
Energy per site obtained via projection on the HF det. of the Gutzwiller ST Hamiltonian on a 256-site lattice and in the TDL compared with AFQMC results[5]

| | $U/t = 2$ | | $U/t = 4$ | | $U/t = 6$ | | $U/t = 8$ | |
|---|---|---|---|---|---|---|---|---|
| | PBC | APBC | PBC | APBC | PBC | APBC | PBC | APBC |
| $E_{ref}$ | -1.174203(23) | -1.177977(20) | -0.86051(16) | -0.86055(16) | -0.65699(12) | -0.65707(20) | -0.52434(12) | -0.52441(12) |
| $E_J$ | -1.151280 | -1.166370 | -0.76354 | -0.77769 | -0.42855 | -0.44160 | -0.12848 | -0.14051 |
| $J_{opt}$ | -0.29233 | -0.28957 | -0.56284 | -0.55787 | -0.80107 | -0.79460 | -1.00701 | -0.99956 |
| $E_J/E_{ref}\%$ | 98.0 | 99.0 | 88.7 | 90.4 | 65.3 | 67.2 | 24.5 | 26.8 |
| $E_{ref}^{TDL}$ | -1.1760(2) | | -0.8603(2) | | -0.6567(3) | | -0.5243(2) | |
| $E_J^{TDL}$ | -1.1609 | | -0.7686 | | -0.4203 | | -0.0943 | |
| $J_{opt}^{TDL}$ | -0.29025 | | -0.55911 | | -0.79621 | | -1.00142 | |
| $E_J^{TDL}/E_{ref}\%$ | 98.7 | | 89.4 | | 64.0 | | 18.0 | |

- **ST results** based on a single det. recover **>85%** of correlation energy for $U/t$ up to 4.

**More compact wavefunction:**

- Left and right eigenvector of non-hermitian Hamiltonian differ.
- Right eigenvector sparser than original, while left eigenvector more diperse.
- Optimal J determined by projection close to maximum in $L_2$ norm.

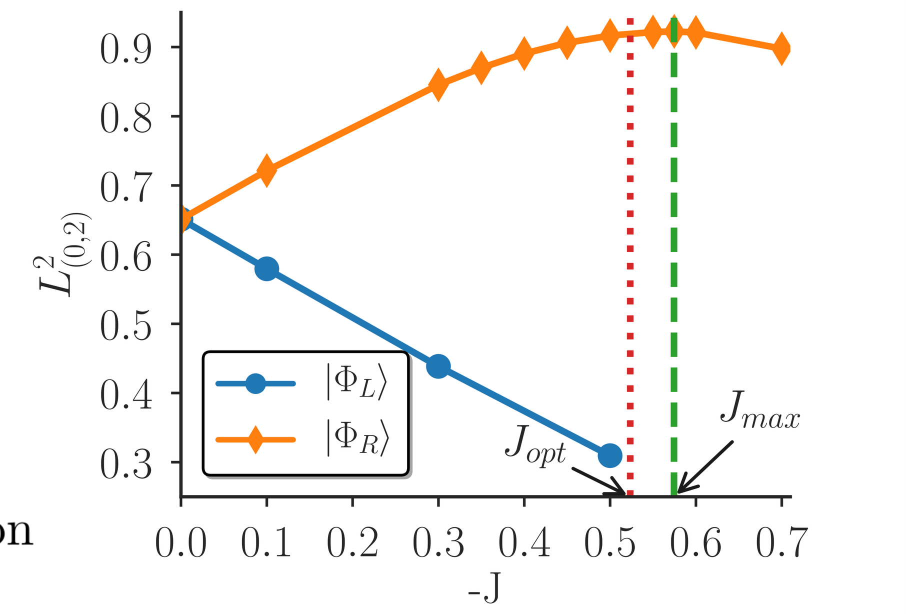



(a) $L_2$ norm inside doubles of left and right EV. (b) HF, VMC and variance minimization energy of a 6-site chain at U = 4.

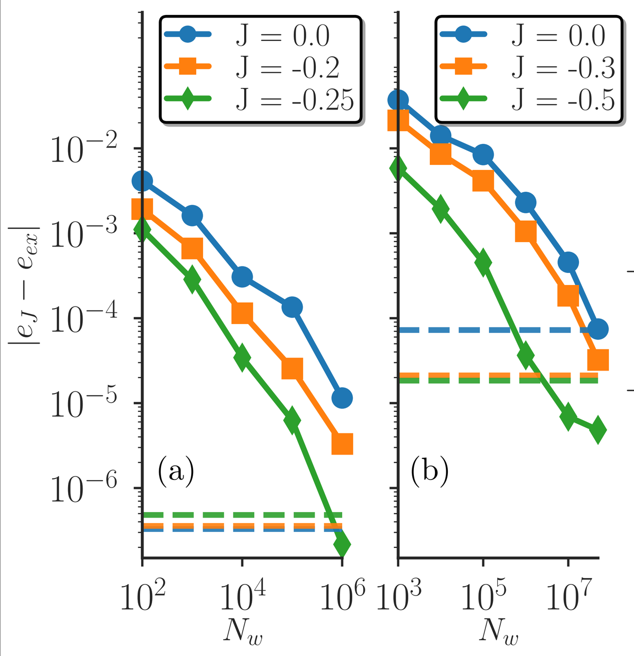
## Gutzwiller ST-FCIQMC results in momentum-space

**18-site half-filled Hubbard model up to $U/t = 4$:**

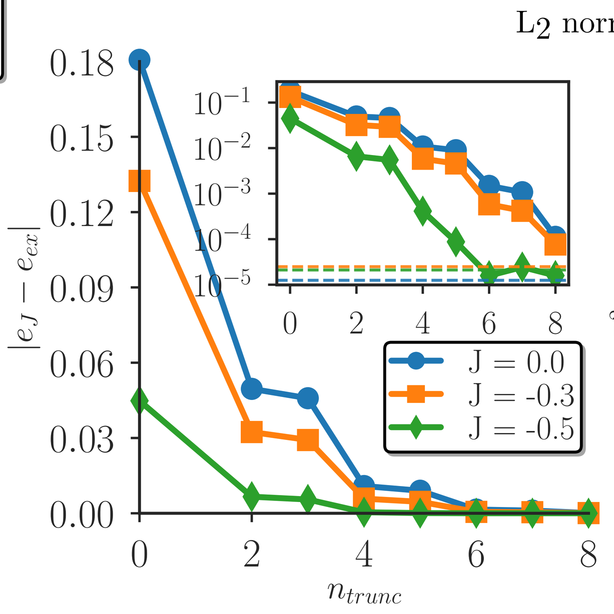
- Benchmark system with exact result available
- Total Hilbert space size: ~147M
- Huge *energy improvement* comp. to standard FCIQMC
- Good agreement with $E_{ex}$ already at CISDTQ
- *More compact* form of GS wave function



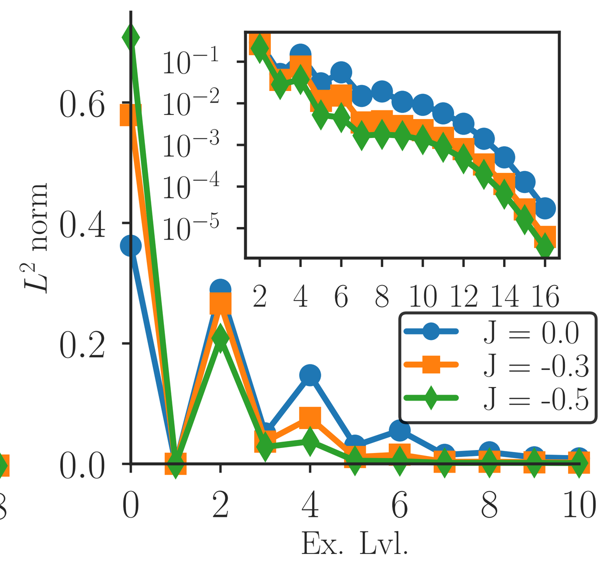

$L_2$ norm inside doubles vs. J




Error in energy vs. walker number.
(a) U/t = 2, (b) U/t = 4.




Error vs. exc. lvl. trunc., U/t = 4.




$L_2$ norm per excitation level

**50-site lattice:**

- *huge improvement* to standard FCIQMC
- *good agreement* with AFQMC reference results
- even *off half-filling*

Comparison of the effect of ST with AFQMC[4,5] in the 50-site lattice

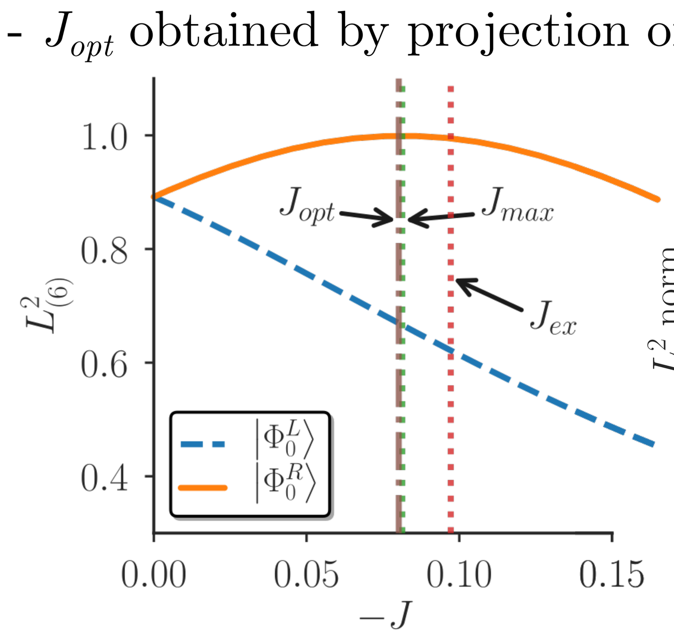
| $U/t$ | $n_{el}$ | AFQMC | iFCIQMC | iST-FCIQMC | $\Delta E_{ST}$ |
|---|---|---|---|---|---|
| 1 | 50 | -1.43718(11) | -1.4371801(18) | -1.43724130(44) | -0.00006(11) |
| 2 | 50 | -1.22278(17) | -1.220590(16) | -1.2228426(80) | -0.00006(18) |
| 3 | 50 | -1.03460(30) | -1.023064(35) | -1.034788(18) | -0.00019(32) |
| 4 | 50 | -0.879660(20) | -0.83401(15) | -0.880657(60) | -0.000997(80) |
| 4 | 48 | -0.93720(15) | -0.89610(12) | -0.93642(40) | 0.00078(55) |
| 4 | 46 | -0.9911420(86) | -0.95550(15) | -0.990564(89) | 0.00058(18) |
| 4 | 44 | -1.037883(59) | -1.006483(38) | -1.037458(47) | 0.00043(11) |
| 4 | 42 | -1.079276(66) | -1.053756(64) | -1.078908(69) | 0.00037(14) |

## Hopping ST-FCIQMC results in real-space

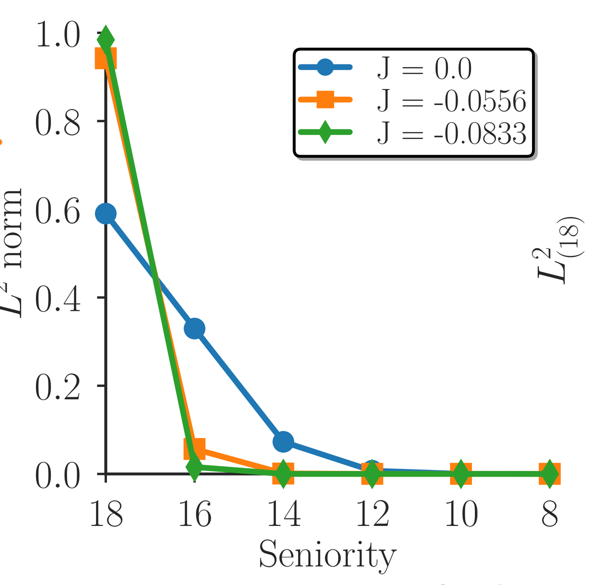
- Anti-ferromagnetic **Neel-state** reference in the large $U/t$ regime
- **Long-range** *one-* and *two*-body interactions, due to ST:

$$F(J', \mathbf{i}, \mathbf{j}, \mathbf{k}, \mathbf{l}) = \sum_{\mathbf{m}} G(J', \mathbf{i} - \mathbf{m}) G(J', \mathbf{j} - \mathbf{m}) G(-J', \mathbf{m} - \mathbf{k}) G(-J', \mathbf{m} - \mathbf{l}), \quad G(J', \mathbf{r}) = \frac{1}{M} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} e^{-J'\epsilon(\mathbf{p})}$$

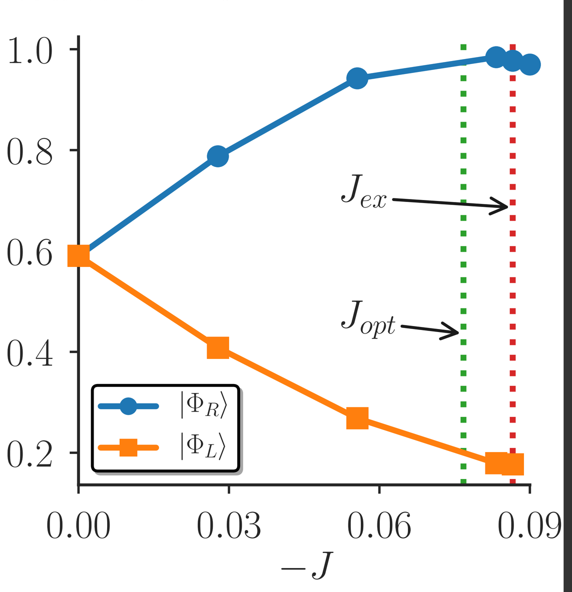
- Right eigenvector concentrated in the **fully open-shell** sector of Hilbert space corresponding to *low energy Heisenberg*-like sector
- $J_{opt}$ obtained by projection on Neel-state *close to maximum* of norm




$L_2$ norm of the all-open-shell states of the exact solution of the half-filled 6-site chain at $U/t$=12.




$L_2$ norm vs. seniority for the 18-site system at $U/t = 12$.




$L_2$ norm in all-open-shell states for the 18-site system at $U/t = 12$.

## Summary & Outlook

**Gutzwiller correlator** in momentum-space representation:

- Huge **energy improvement** and **more compact** form of the GS wavefunction with *managable additional* cost due to 3-body term
- Application to *larger* lattice sizes and *stronger* on-site repulsion $U$ in future.
- Calculation of *excited states* and *other observables* through left-eigenvector

$$\langle \Phi_L | \bar{O} | \Phi_R \rangle = \langle \Psi | e^{\hat{\tau}} e^{-\hat{\tau}} \hat{O} e^{\hat{\tau}} e^{-\hat{\tau}} | \Psi \rangle = \langle \hat{O} \rangle$$

- Detailed study of the **hopping correlator** in real-space for large $U/t$

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