Linear-time generalized Hartree-Fock algorithm for quasi-one-dimensional systems

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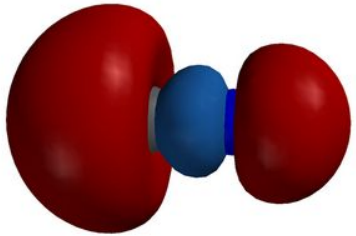
Hartree-Fock

- Common method in *ab initio* chemistry simulations
  - In use for over 70 years
  - Usually accompanied by many corrections to achieve chemical accuracy
- Self-consistent field
- Variational method using Slater determinants,
  - appropriate for repulsive fermions
- Can be generalized to *Gaussian* states
- Permits attractive interactions – related to BCS, BdG theories

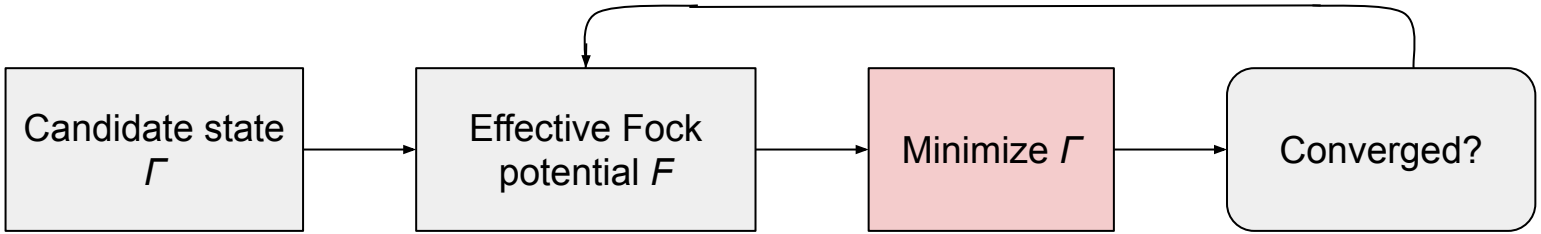


Hartree-Fock

- Amounts to repeated Taylor expansion of quadratic potential:

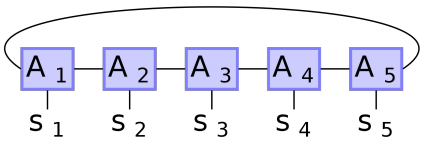
$$\langle \Gamma | \hat{\mathcal{H}} | \Gamma \rangle \approx \text{const.} + \sum \underbrace{\left[T_{ij} + 6 U_{ijk\ell} \Gamma^0_{k\ell} \right]}_{F_{ij}} \Gamma_{ij}$$

- Eigendecomposition: $O(N^3)$ operations on N sites (spin-orbitals)



Matrix Product States

- MPS: Efficient representation in quasi-1D systems
- For entanglement E, reduces memory from 2^N to $N \times 2^E$
- Optimize on a *k*-local Hamiltonian with DMRG

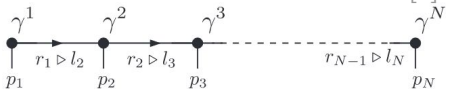


DMRG takes O(n) time for fixed entanglement

(Gaussian Fermionic) Matrix Product States

- Gaussian MPS: adaptation of MPS to store Gaussian states
- For entanglement E, reduces memory from N^2 to $N \times E^2$
- Optimize on a *k*-local quadratic Hamiltonian with GFMPS-DMRG

[3]



$O(N^3)$ Eigendecomposition replaced by O(N) GFMPS DMRG

1: *Gaussian Matrix Product States*, Norbert Schuch, Michael M. Wolf, J. Ignacio Cirac, arXiv:1201.3945

2: *Compression of correlation matrices and an efficient method for forming matrix product states of fermionic Gaussian states*, Matthew T. Fishman and Steven R. White, Phys. Rev. B 92, 075132

3: *Matrix product state algorithms for Gaussian fermionic states*, Norbert Schuch and Bela Bauer, Phys. Rev. B 100, 245121

Numerical Experiments

What accuracy can we expect? How many gHF iterations, DMRG sweeps, bond dimension is necessary?

Test on rectangular, inhomogeneous Hubbard model:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}} + \hat{\mathcal{H}}_{\text{trap}}$$

$$\hat{\mathcal{H}}_0 = -t \sum_{\langle \mathbf{x},\mathbf{y} \rangle, \sigma} \hat{a}^\dagger_{\mathbf{x}\sigma} \hat{a}_{\mathbf{y}\sigma} - \mu \sum n_{\mathbf{x}\sigma}$$ ← Hopping terms

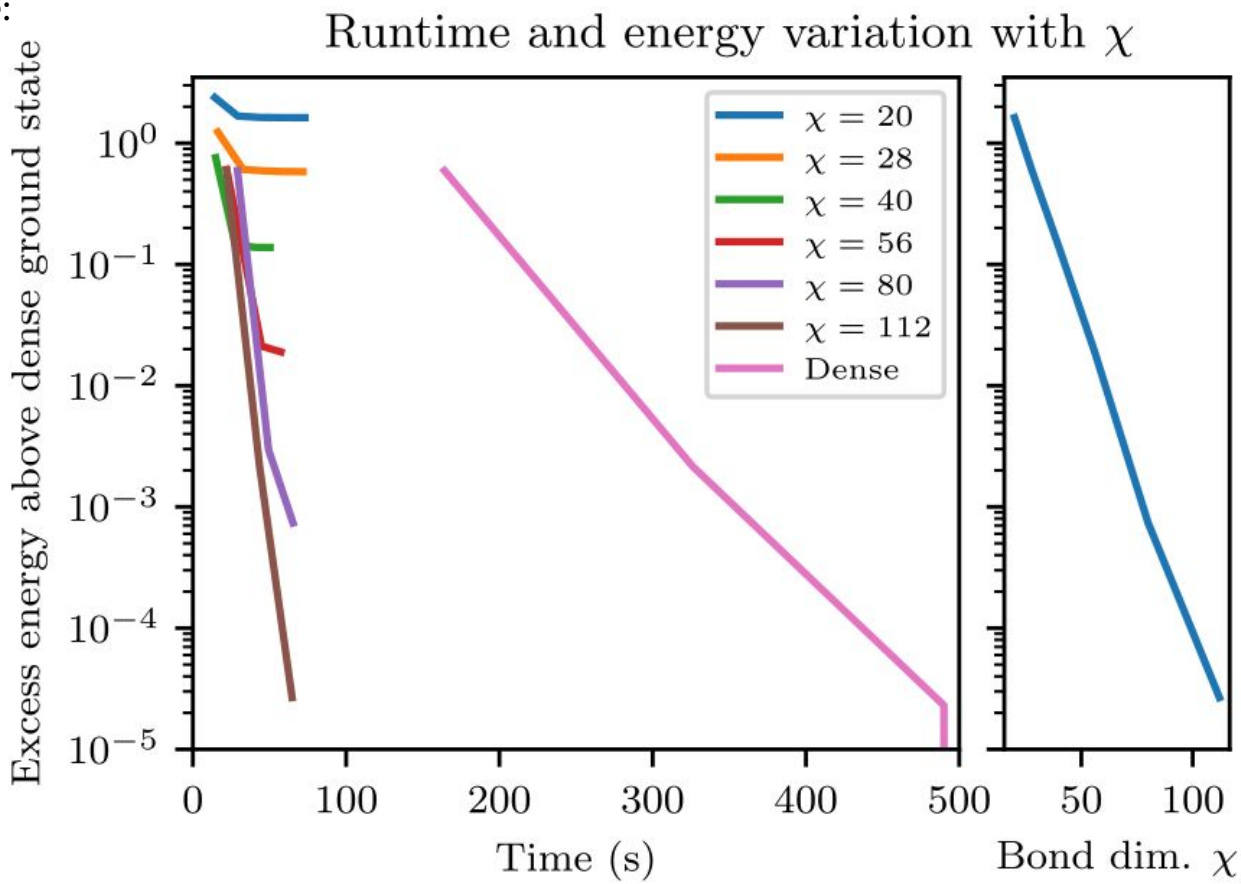
$$\hat{\mathcal{H}}_{\text{int}} = U \sum_{\mathbf{x}} \left(\hat{n}_{\mathbf{x}\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{x}\downarrow} - \frac{1}{2} \right)$$ ← On-site repulsion

$$\hat{\mathcal{H}}_{\text{trap}} = \sum_{x,y,\sigma} (V_x x^2 + V_y y^2) \hat{n}_{x,y,\sigma}$$ ← Quadratic potential

Quadratic “trap” potential loosely models trapped quantum gas scenarios

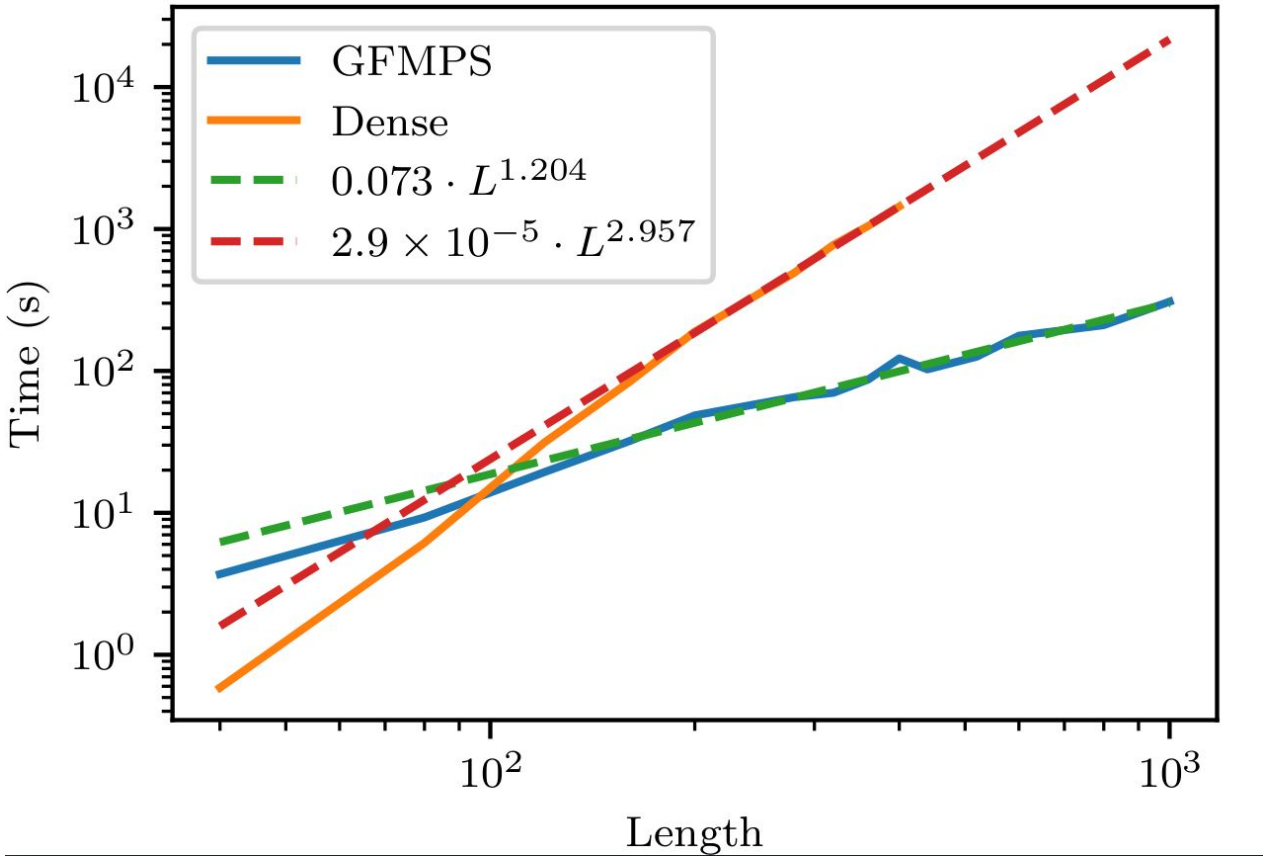
4x280 Rectangular Hubbard Model

Weakly repulsive:
$U = 0.4t$
$\mu = 0.3t$



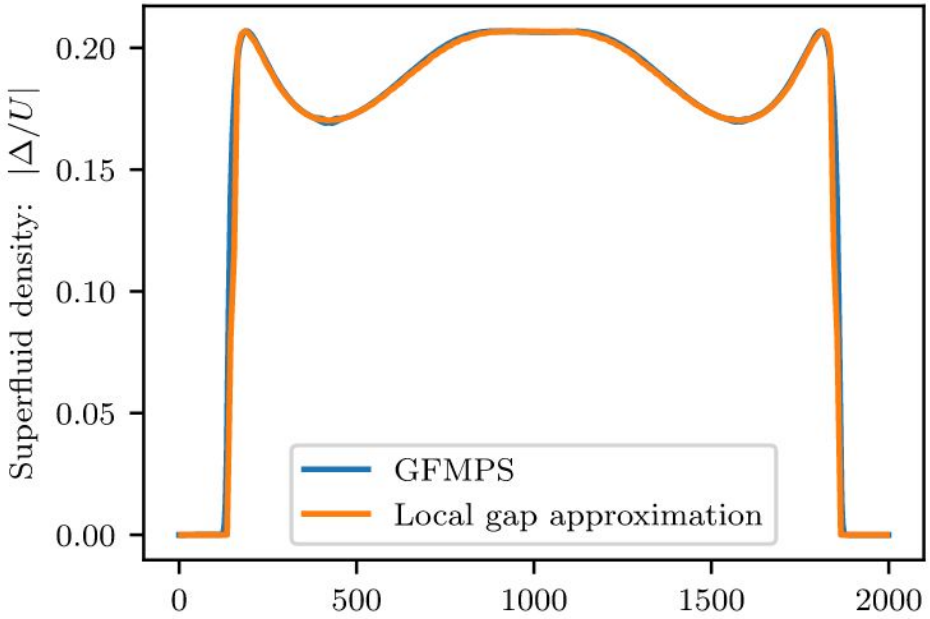
4×L: Linear Scaling in System Size

Weakly repulsive:
$U = 0.4t$
$\mu = 0.3t$



4x2000: Attractive Case

Strongly attractive: $U = -3.0t$, $\mu = -1.0t$, still with quadratic trapping potentials

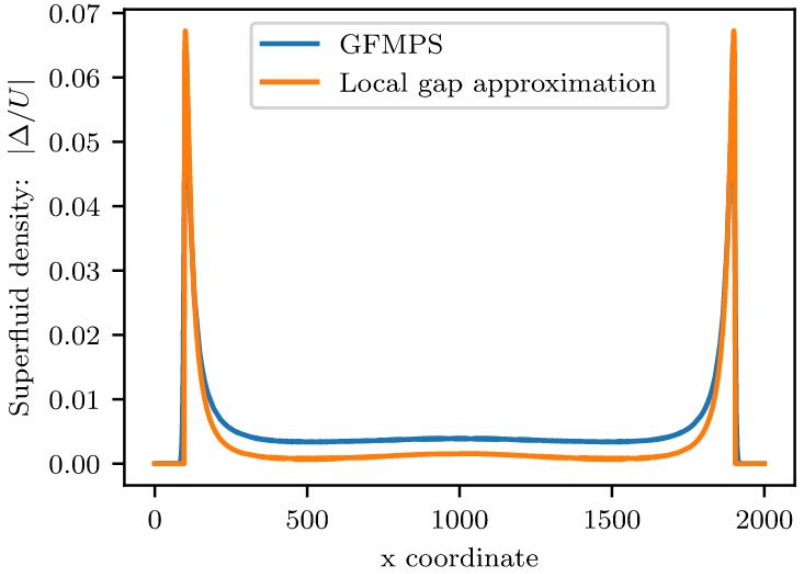


Local BCS theory predicts a gap Δ(U, μ) at each site.

Forms an accurate model when coherence length is short (< 10 sites)

4x2000: Attractive Case

Weakly attractive: $U = -0.65t$, $\mu = -0.75t$, still with quadratic trapping potentials



Local approximation becomes very inaccurate when coherence length grows.
Off by factor of 2 even on 2000 site system!
gHF-GFMPS allows us to probe superconducting effects in this regime

Thank you!

Gaussian States

- Any Fermionic state ρ has associated covariance matrix:

$$\Gamma_{ij} = \frac{i}{2}\,\mathrm{Tr}(\rho[\hat{c}_i, \hat{c}_j]) \qquad \Gamma^2 = -\mathbb{1}$$

- Gaussian states: fully defined by this matrix
- Γ gives 2-operator expectations
- Gaussianity gives all *n*-way expectations: Wick's Theorem

$$\langle \hat{c}_i \hat{c}_j \hat{c}_k \hat{c}_l \rangle = \langle \hat{c}_i \hat{c}_j \rangle \langle \hat{c}_k \hat{c}_l \rangle - \langle \hat{c}_i \hat{c}_k \rangle \langle \hat{c}_j \hat{c}_l \rangle + \langle \hat{c}_i \hat{c}_l \rangle \langle \hat{c}_j \hat{c}_k \rangle$$

Gaussian States: 2-operator interactions

Given a Hamiltonian quadratic in fermionic operators:

$$\hat{\mathcal{H}} = -i \sum_{i,\,j} H_{ij} \hat{c}_i \hat{c}_j$$

Energy of a candidate state:

$$\langle \mathcal{H} \rangle = \mathrm{Tr}[\Gamma H]$$

Efficiently optimized by an eigendecomposition of *H*:

$$\Gamma = i(V_- V_-^\dagger - V_+ V_+^\dagger)$$

V_- (resp V_+) are eigenvectors with negative (resp positive) eigenvaluates

Gaussian States: 4-operator interactions

Sufficient to describe pairwise repulsion (or attraction) between fermions

$$\hat{\mathcal{H}} = -i \sum T_{ij} \hat{c}_i \hat{c}_j + \sum U_{ijk\ell} \hat{c}_i \hat{c}_j \hat{c}_k \hat{c}_l$$

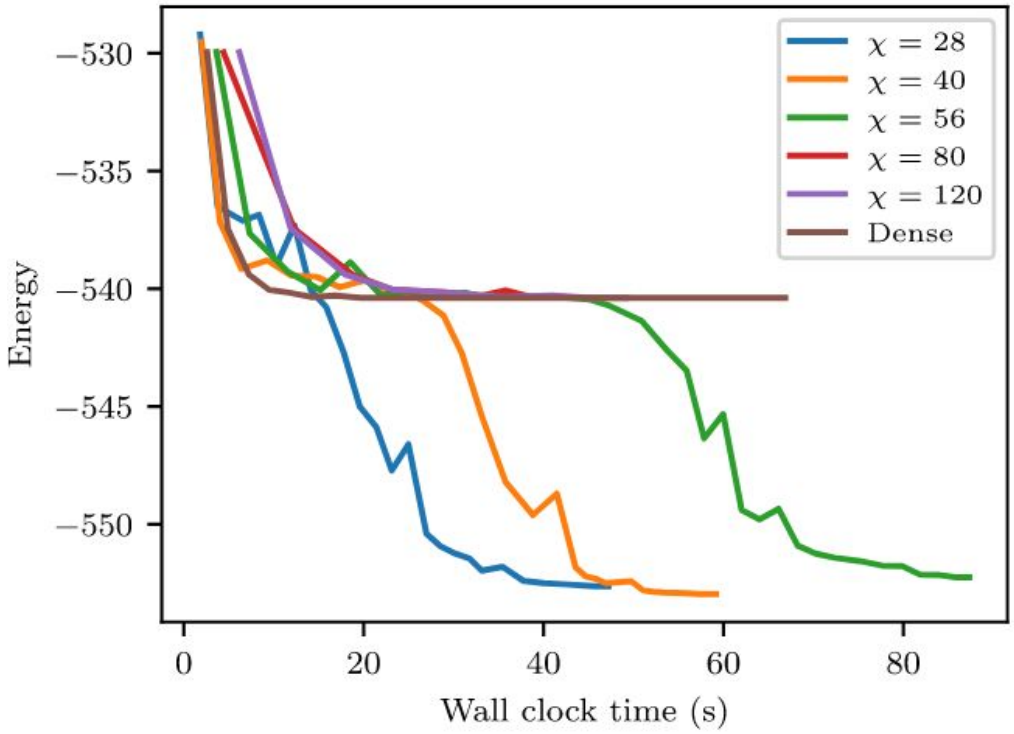
Wick's Theorem says the energy given Γ is:

$$\langle \Gamma | \hat{\mathcal{H}} | \Gamma \rangle = \sum T_{ij} \Gamma_{ij} + 3 \sum U_{ijk\ell} \Gamma_{ij} \Gamma_{kl}$$

Quadratic energy – No efficient solution to exactly minimize over Gaussian states, but…

4x400: Half-Filling Phase Transition

Strongly repulsive: $U = 3.0t$, $\mu = 0.3t$



Higher bond dimension (and dense solution) have early energy plateaus.
Stuck in a local minimum?

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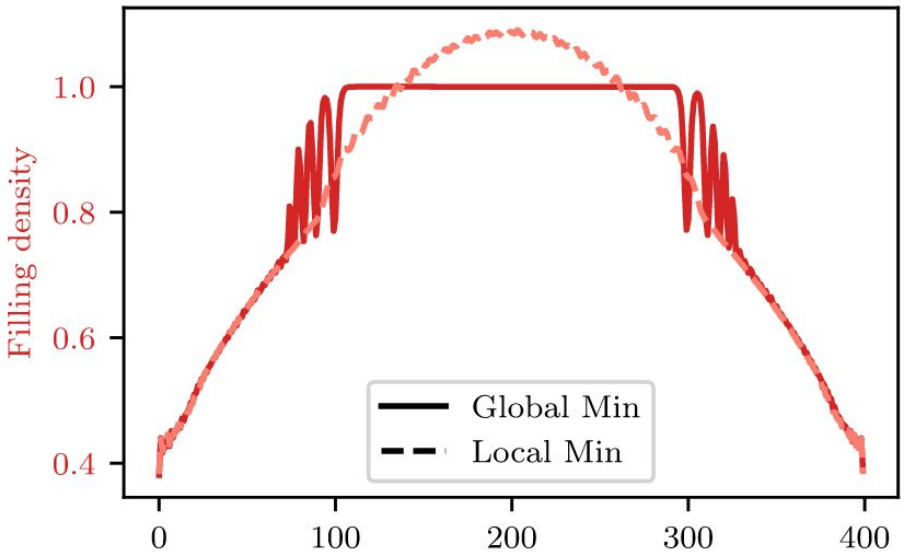
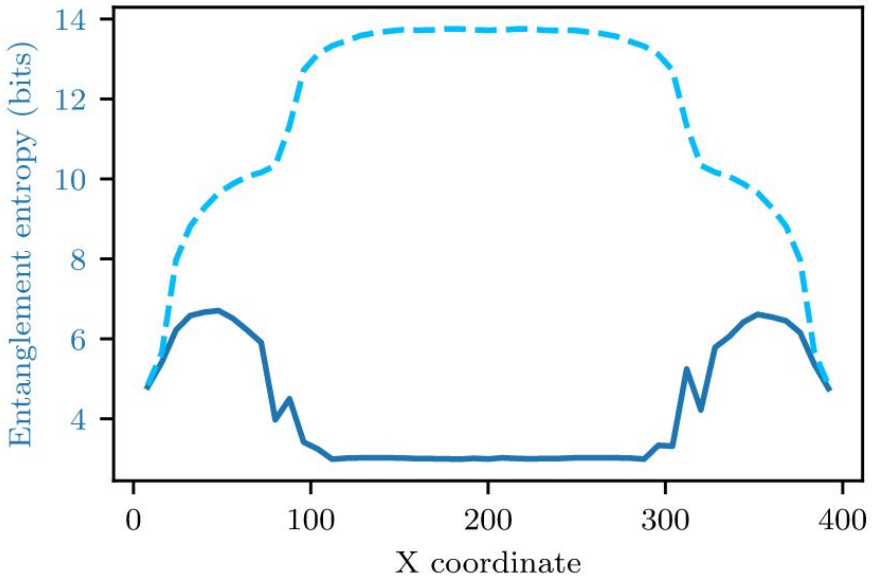
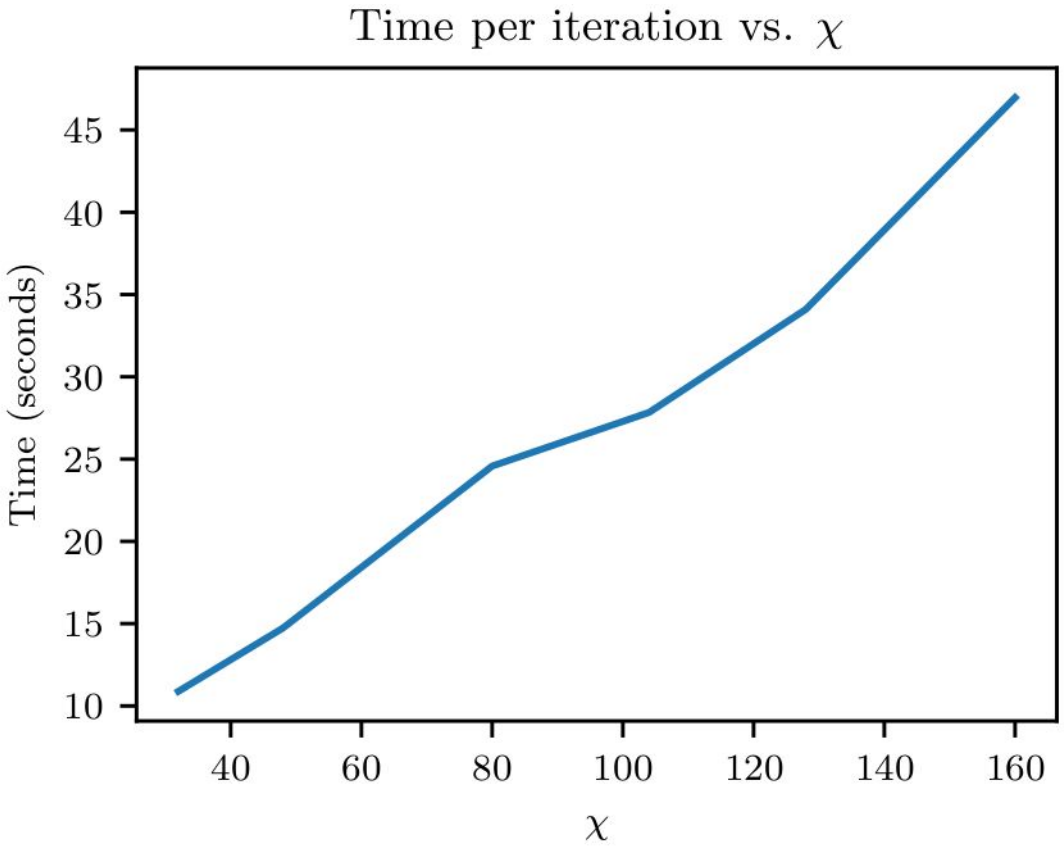




Local minimum: metallic state, high entanglement entropy.
[GFMPS] DMRG favors low entanglement entropy, guides it to half-filling state.
We observe Friedel oscillations near the transition between phases.

4x280: Linear Scaling in Bond Dimension

Weakly repulsive:
$U = 0.4t$
$\mu = 0.3t$



Hartree Fock + GFMPS DMRG

- Generalized Hartree Fock (gHF)[1, 2], closely related to the Bogoliubov-de Gennes equations, BCS ansatz[3]
  - Supports superconducting pairing terms – necessary when interactions are attractive
  - Not to be confused with chemists' "generalized Hartree-Fock", regarding unpaired spins
- Hartree-Fock-type Taylor expansion of quartic interactions, repeated optimization
- Eigendecomposition replaced by much faster GFMPS DMRG

1: Generalized Hartree-Fock theory and the Hubbard model, Volker Bach, Elliott H. Lieb & Jan Philip Solovej, Journal of Statistical Physics volume 76, pages 3–89 (1994)

2: Generalized Hartree–Fock theory for interacting fermions in lattices: numerical methods, Christina V Kraus and J Ignacio Cirac, 2010 New J. Phys. 12 113004

3: BCS ansatz, Bogoliubov approach to superconductivity and Richardson-Gaudin exact wave function, M. Combescot, W. V. Pogosov, O. Betbeder-Matibet, arXiv:1111.4781

Hartree-Fock SPLIT PICTURE

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  - In use for over 70 years
  - Usually accompanied by many corrections to achieve chemical accuracy
- Amounts to repeated Taylor expansion of quadratic potential:

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- Repeatedly compute *F*, optimize Γ (eigendecomposition), repeat until convergence
- Eigendecomposition: $O(N^3)$ operations on N sites (spin-orbitals)
- Storing Γ takes $O(N^2)$ memory. Effectively limits N to ~1000