Recent developments in auxiliary-field quantum Monte Carlo: magnetic orders and spin-orbit coupling

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Collaborators:

- Mingpu Qin
- Peter Rosenberg
- Simone Chiesa
- ***Shiwei Zhang***

Outline

- Introduction to AFQMC
  - Release constraint
  - Symmetry in trial wave function
  - Generalized Hartree–Fock (GHF) wave function
- Magnetic orders in 2D Hubbard model — GHF trial wave function
  - Half-filling: restores symmetry
  - Doped: more accurate results
- Rashba spin-orbit coupling in 2D Fermi gas — GHF random walker
  - Interplay between SOC and interaction
  - Singlet triplet pairing wave function
- Conclusion

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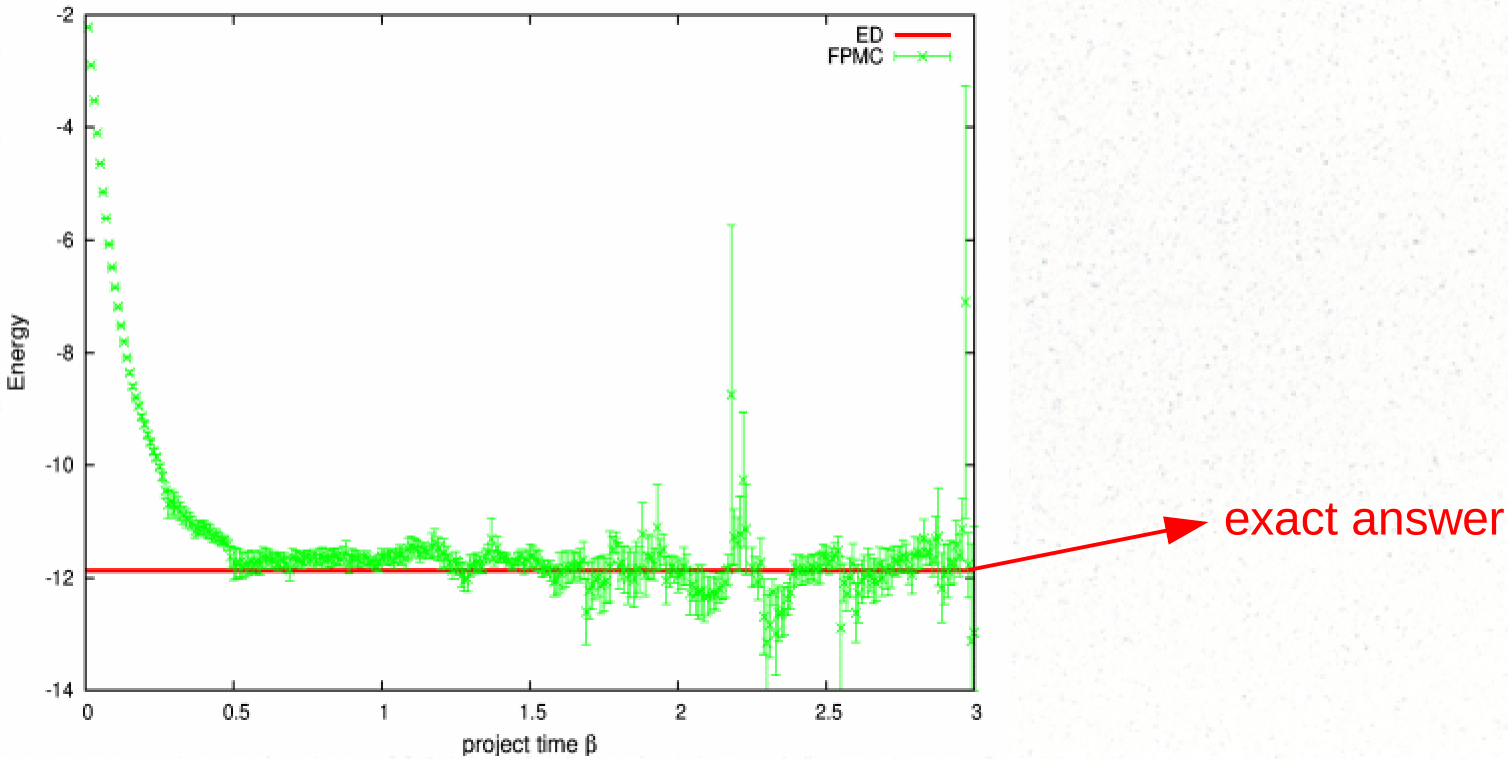
Auxiliary-Field Quantum Monte Carlo

- Random walks in non-orthogonal Slater determinat space
- Scales as N^3 : can simulate large systems
- Systematic error with constraint:
  - highly accurate even with Hartree-Fock trial wave function
- Recently, release constraint, symmetry, Generalized HF: systematically improvable QMC method.

Example

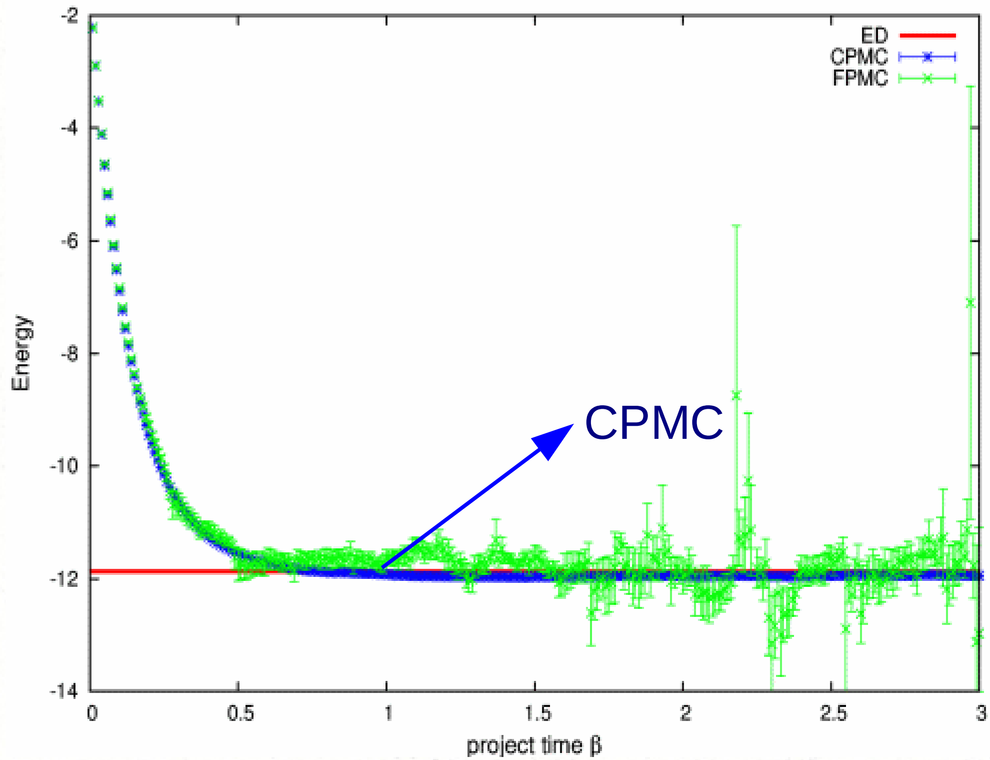
- AFQMC:



Hubbard Model 4x4 7u 7d U=8

Example

- CPMC



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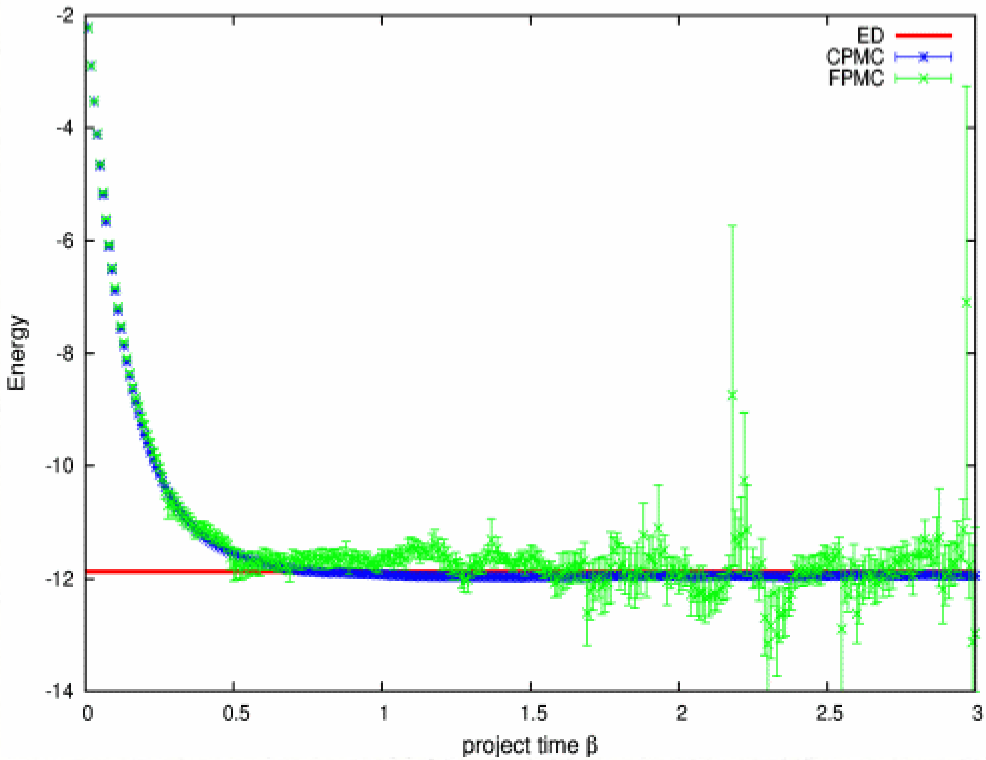

- no sign problem!!

- highly accurate

- much less cpu time
  < 1min on laptop

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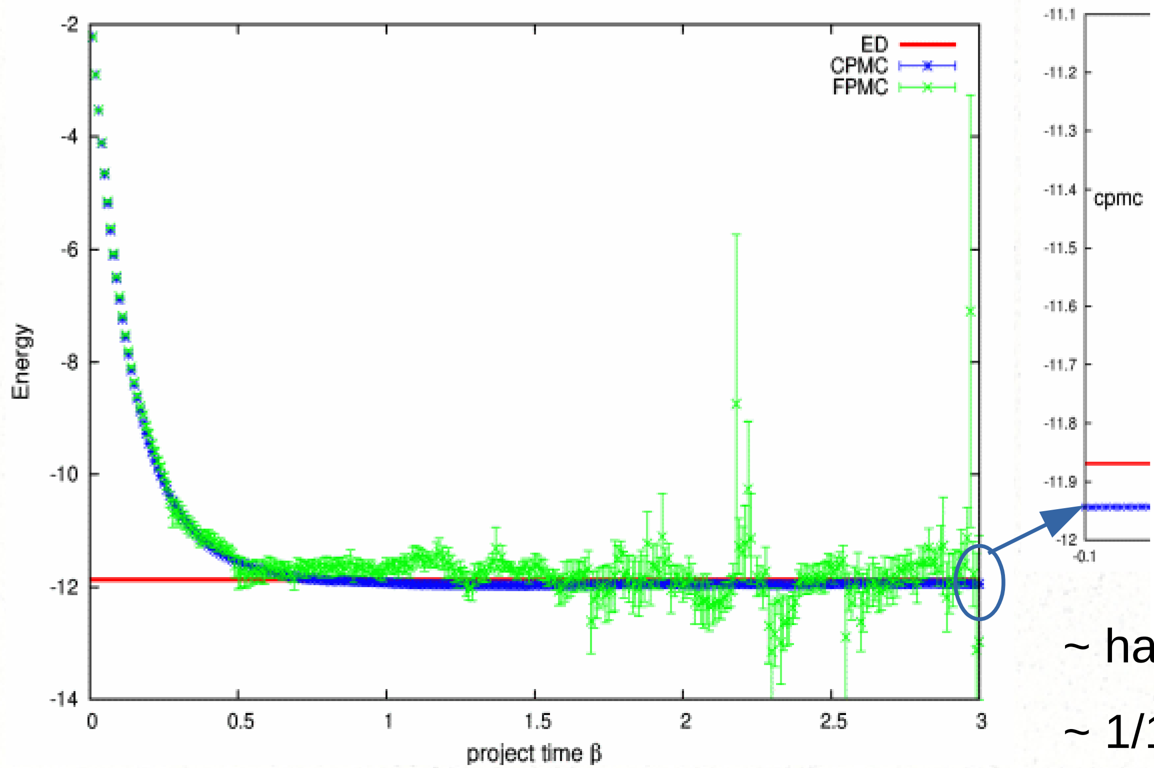
Example

- CPMC



~ half of Trotter error at dt=0.05

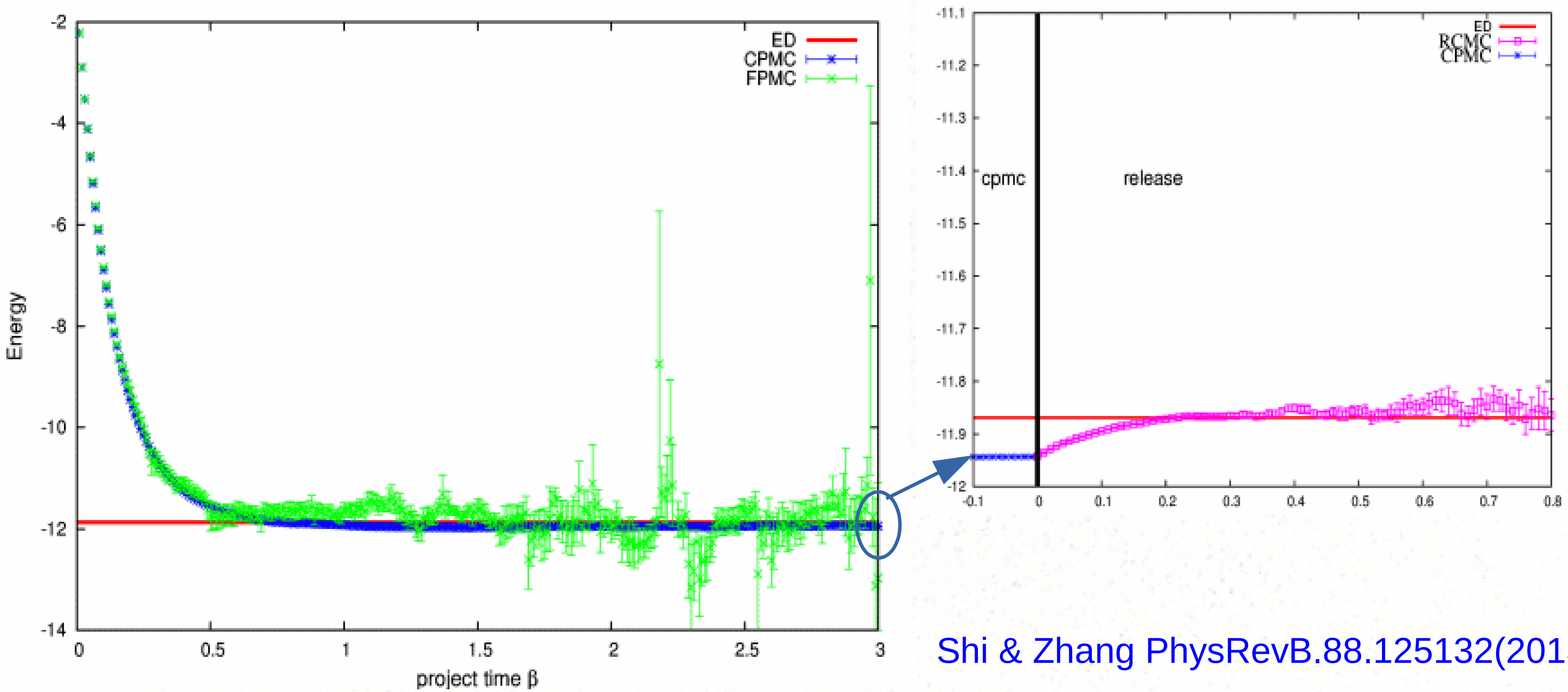
~ 1/10 the error of UCCSD

Hubbard Model 4x4 7u 7d U=8

Example

- Release the constraint

Exact!!! Sign problem!



Shi & Zhang PhysRevB.88.125132(2013)

Hubbard Model 4x4 7u 7d U=8

Symmetry-preserved Wave Functions

- Symmetry for wave function

  Spin in z direction: S_z

PhysRevB.88.125132(2013)

PhysRevB.89.125129(2014)

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PhysRevB.88.125132(2013)

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Symmetry-preserved Wave Functions

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  Spin in z direction: S_z $N_\uparrow$

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Symmetry-preserved Wave Functions

- Symmetry for wave function

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  Total spin: S^2

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Symmetry-preserved Wave Functions

- Symmetry for wave function

Spin in z direction: S_z $N_\uparrow$

Total number of particles: N $N_\downarrow$

Total spin: S^2

Linear Momentum: K

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  -Closed shell system in Hubbard model: symmetry

  -S_z and N are natural for UHF trial wave function

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Symmetry-preserved Wave Functions

- Symmetry for wave function

  Spin in z direction: S_z $N_\uparrow$

  Total number of particles: N $N_\downarrow$

  Total spin: S^2

  Preserve symmetry in projection!

  Linear Momentum: K

  Space group: rotation, mirror, ...

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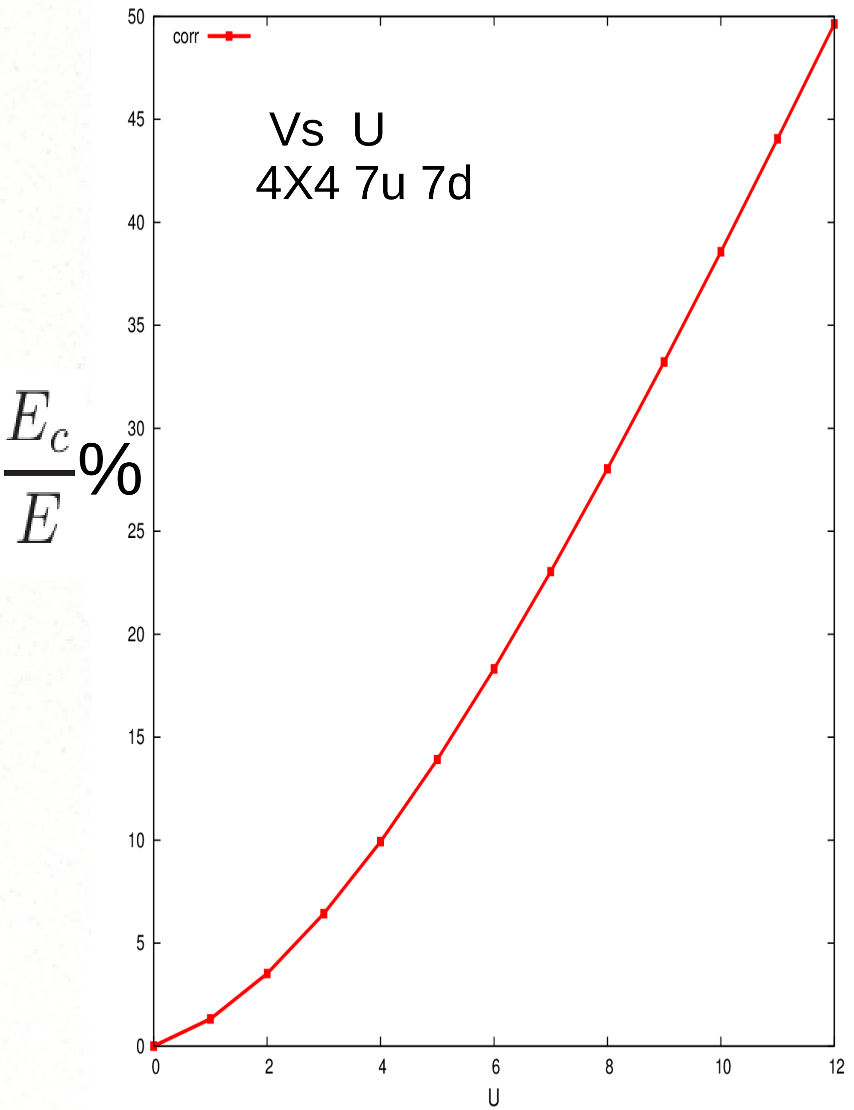
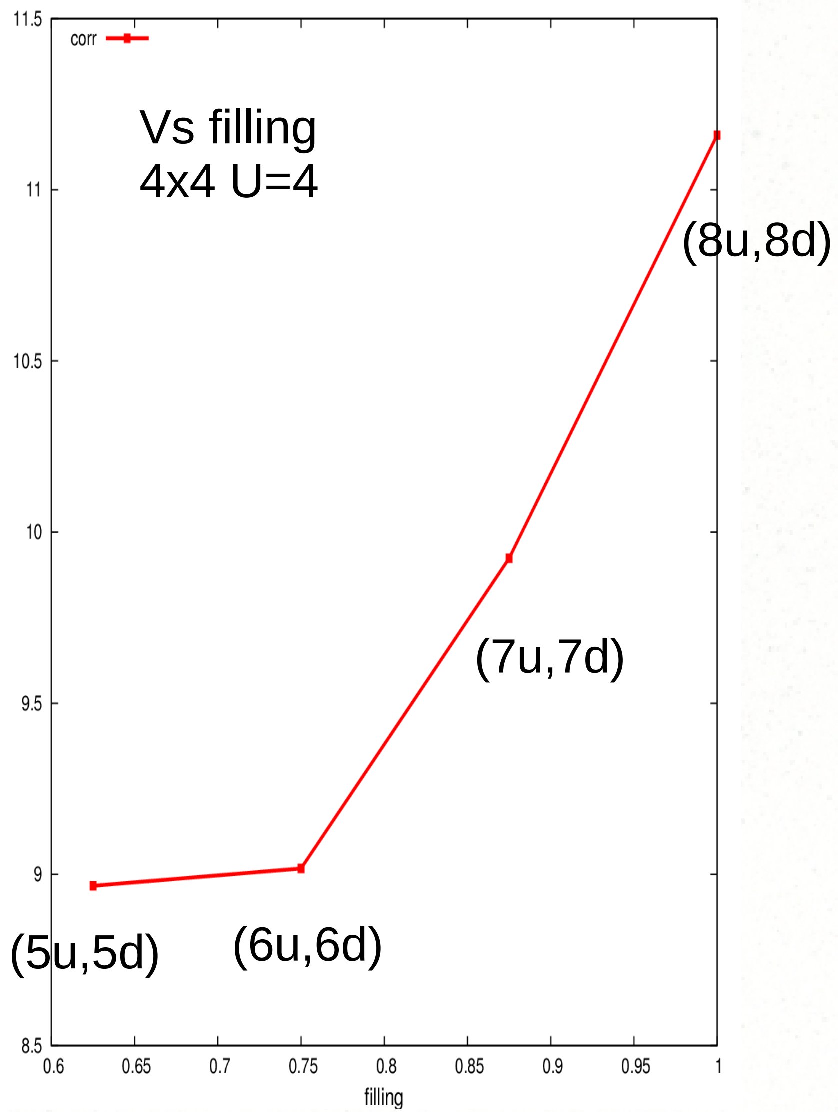
Strongly Correlated Regime





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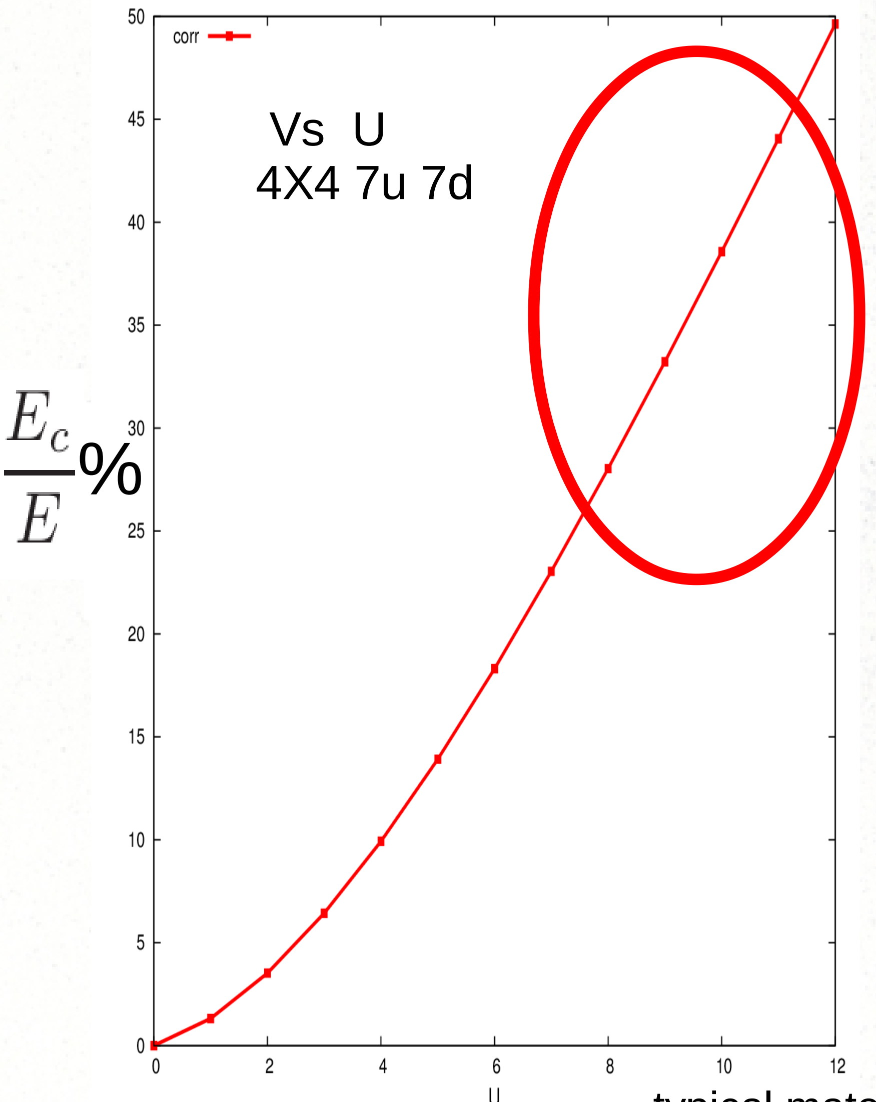
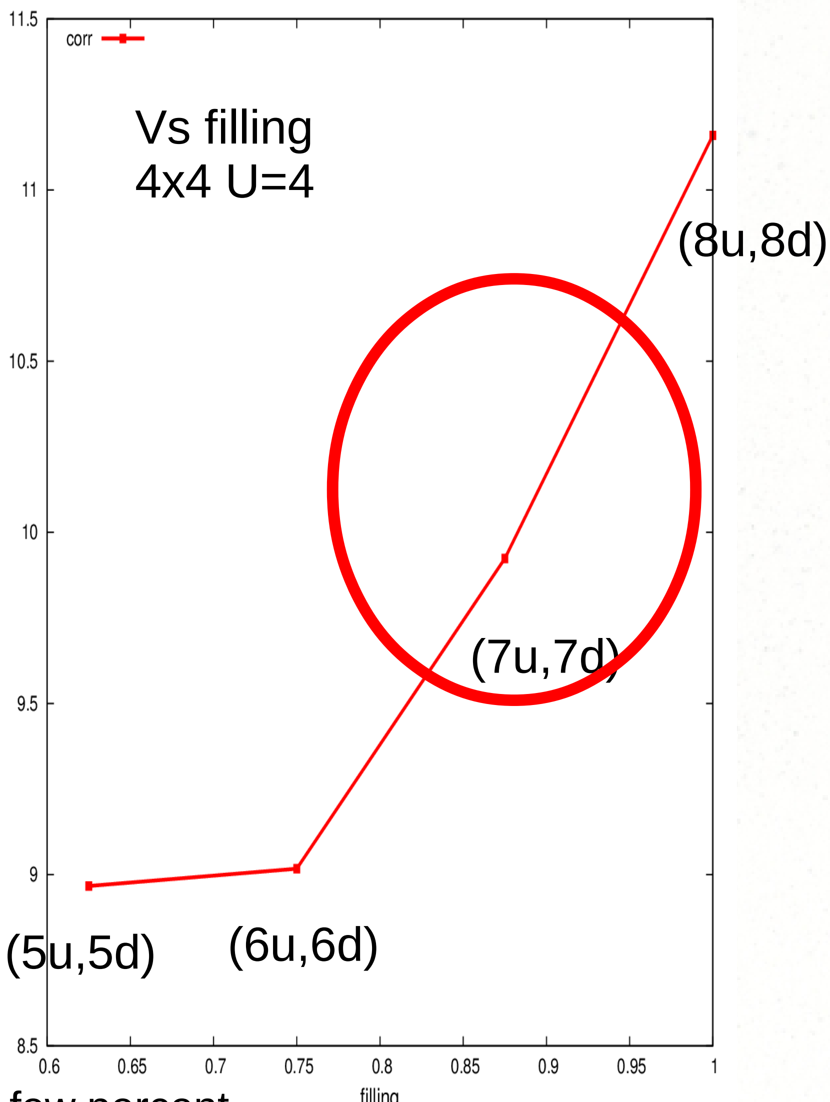


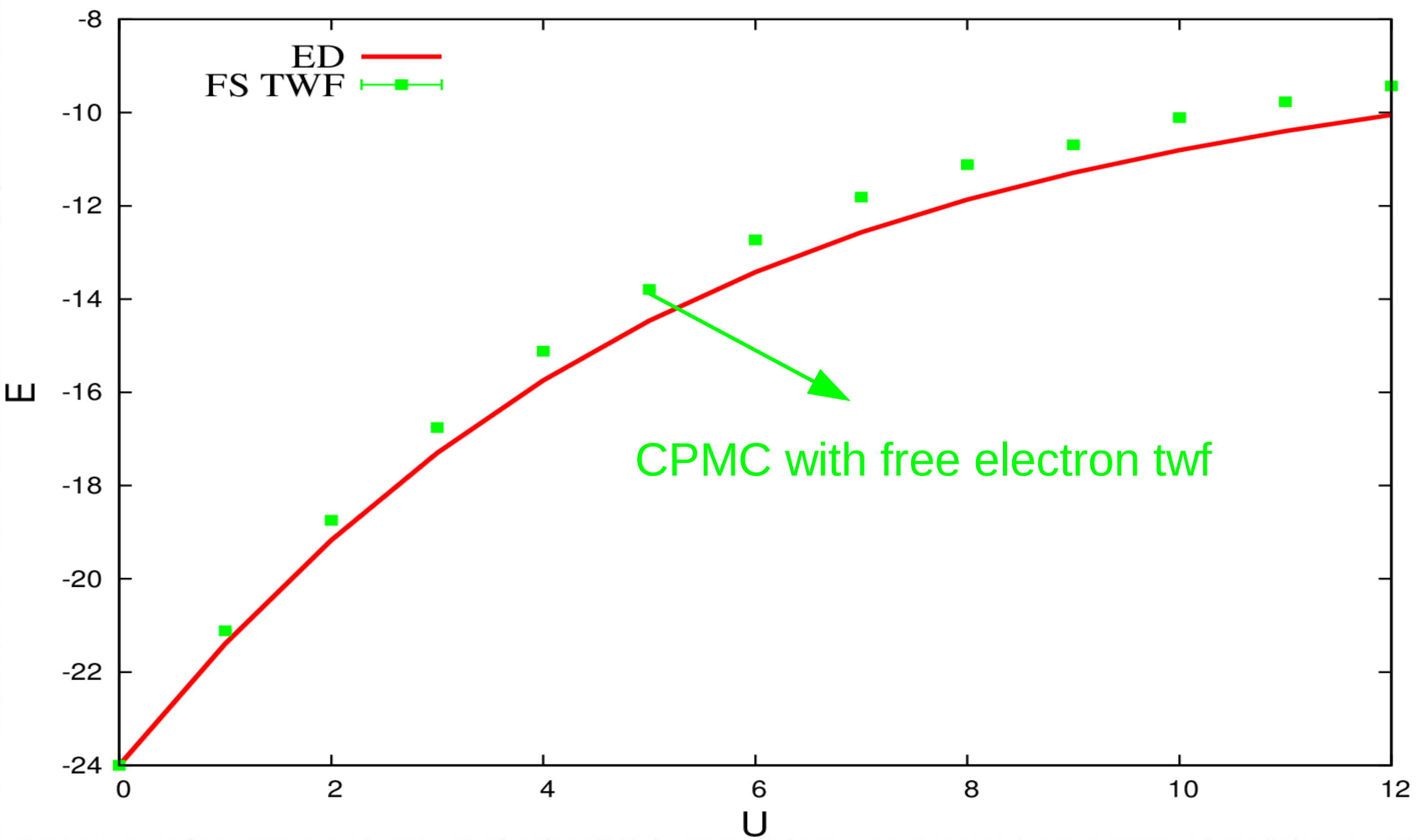


typical material: a few percent

Symmetry in Trial Wave Function

- Large U, highly accurate results

Strongly correlated



open shell

symmetry twf improves results

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CPMC

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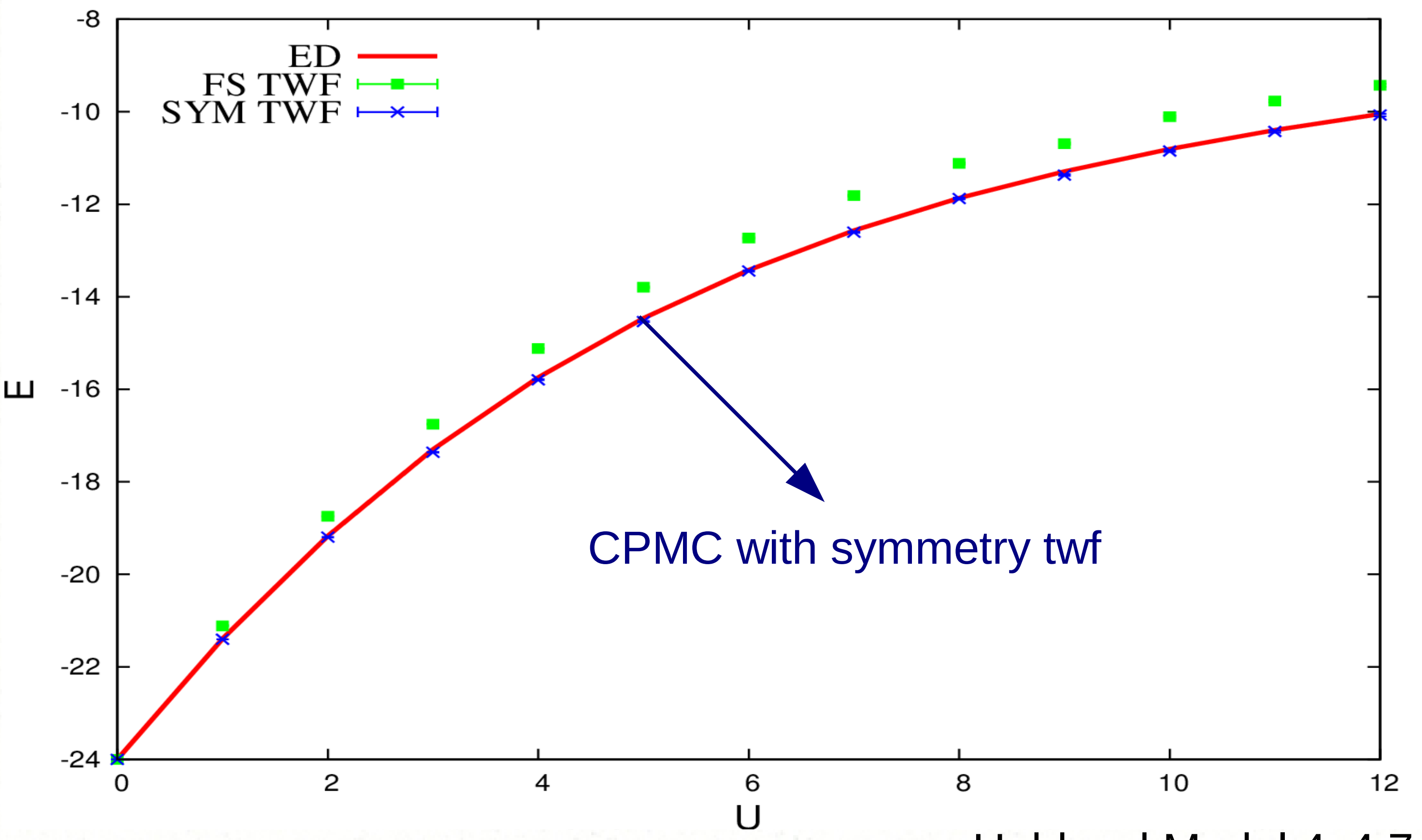

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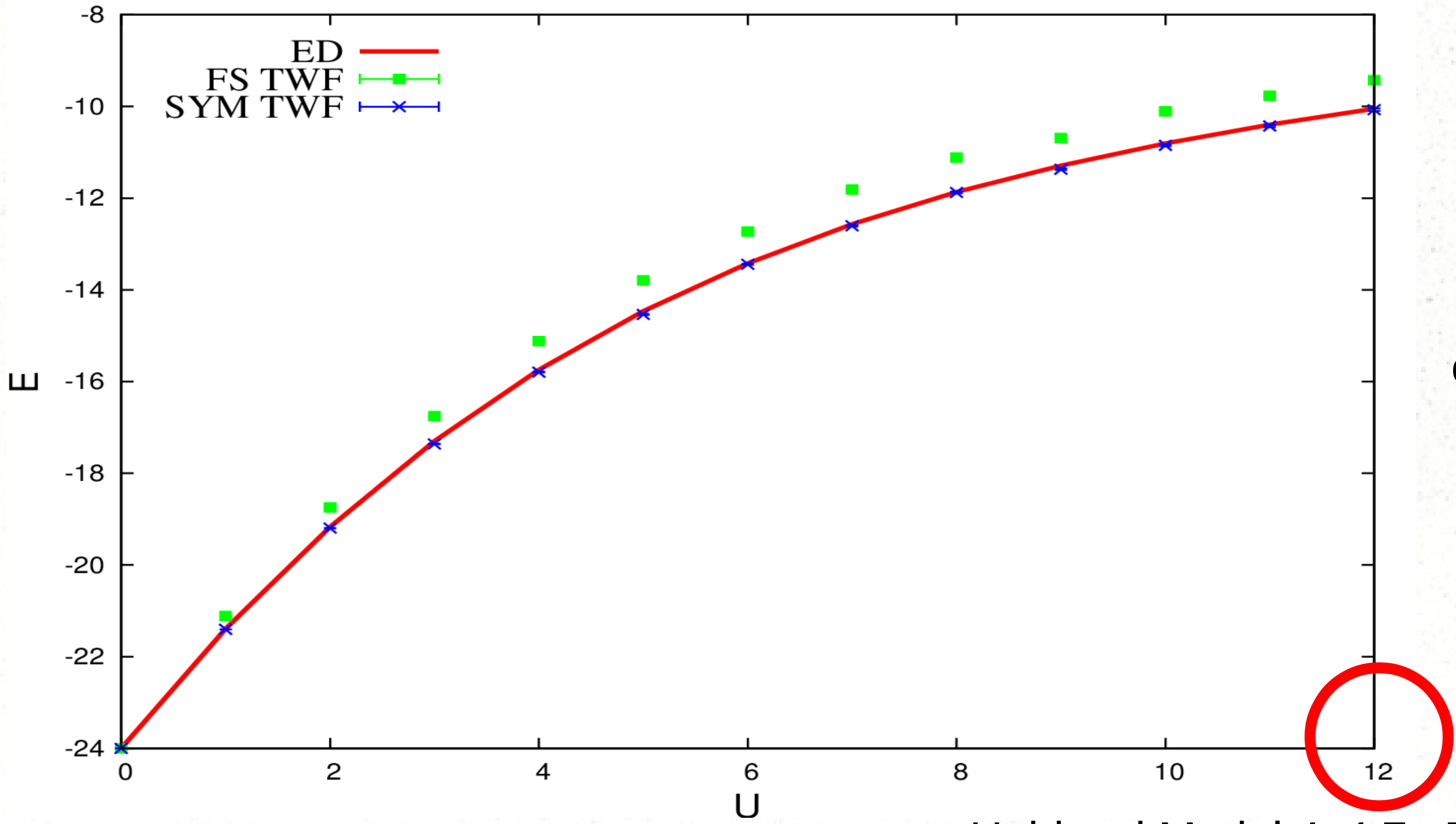
Symmetry in Trial Wave Function

- Large U, highly accurate results correlation energy~50%



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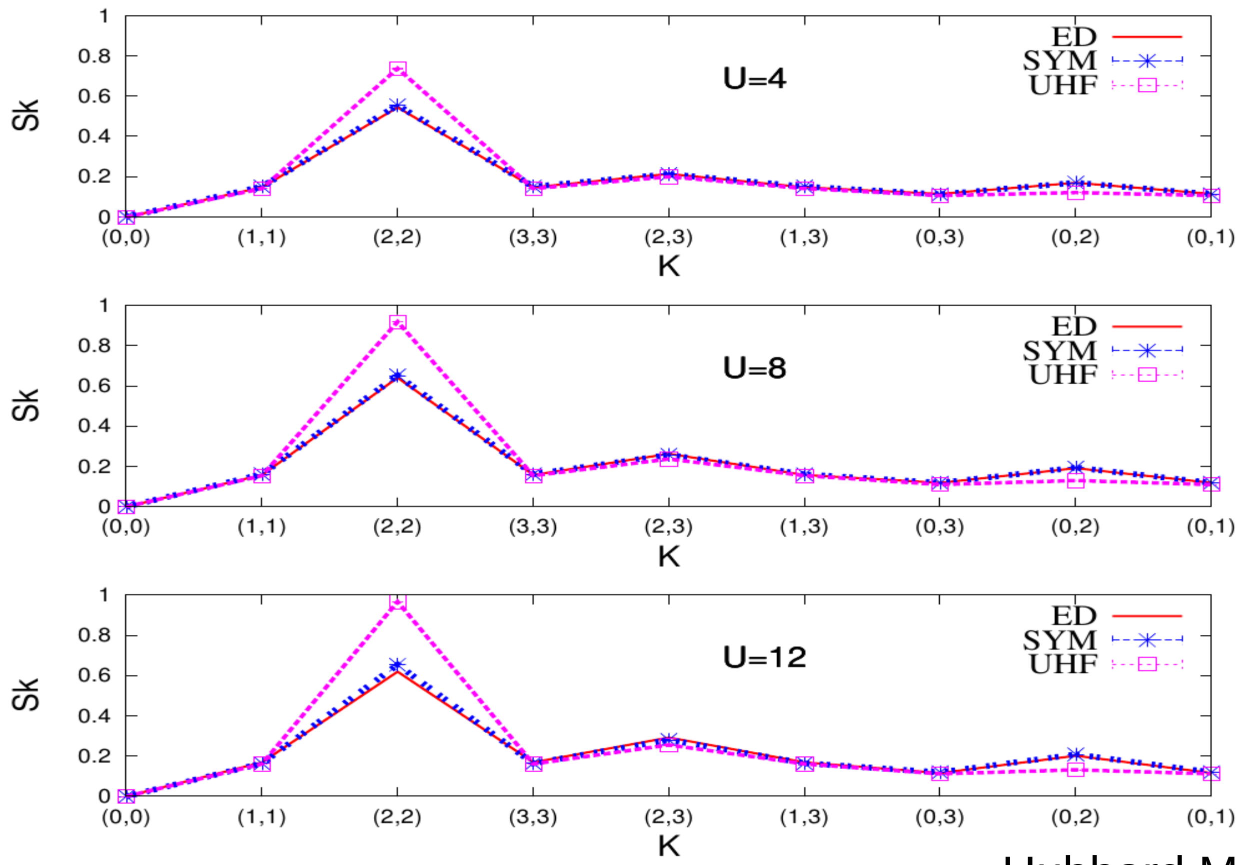
Symmetry in Trial Wave Function

- spin structure factor $S(K) = 1/N \sum_{ij} S_i^z S_j^z \exp[\imath K(R_i - Rj)]$



recover AFM oder

Shi & Zhang
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Generalized HF Trial Wave Function

- Release constraint: exponential scaling
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$$\begin{pmatrix} \psi_1 & \psi_1 & \vdots & \vdots \\ \psi_2 & \psi_2 & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \psi_L & \psi_L & \vdots & \vdots \end{pmatrix}$$

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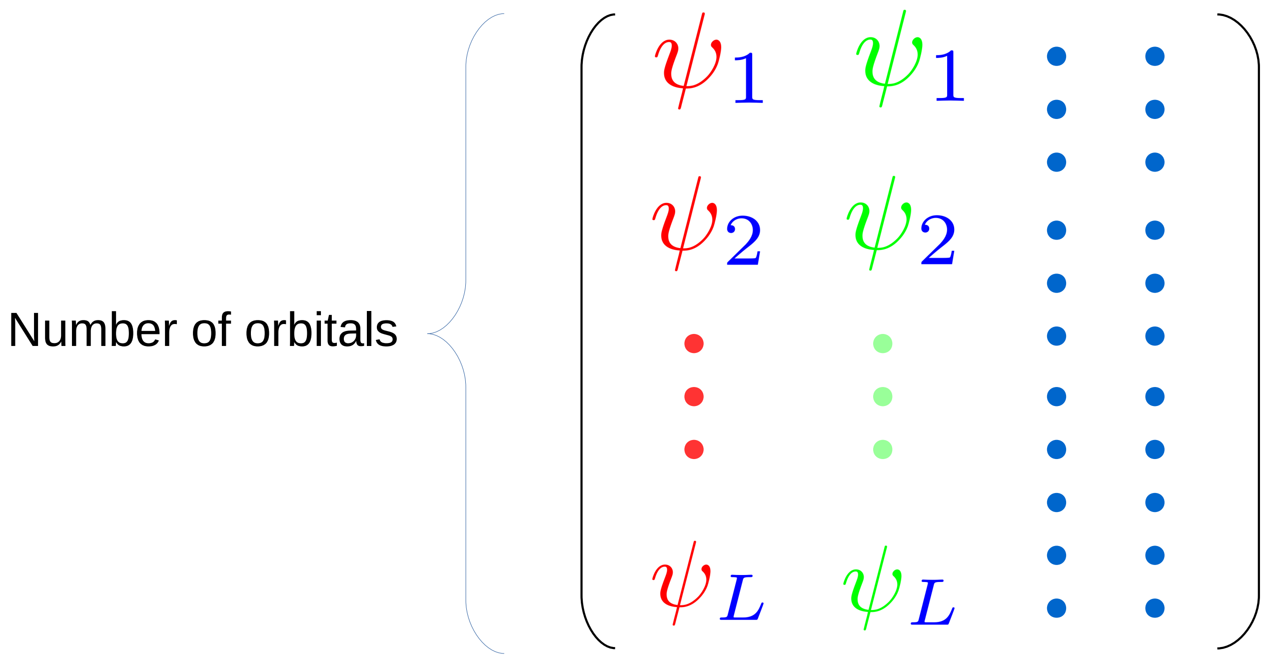

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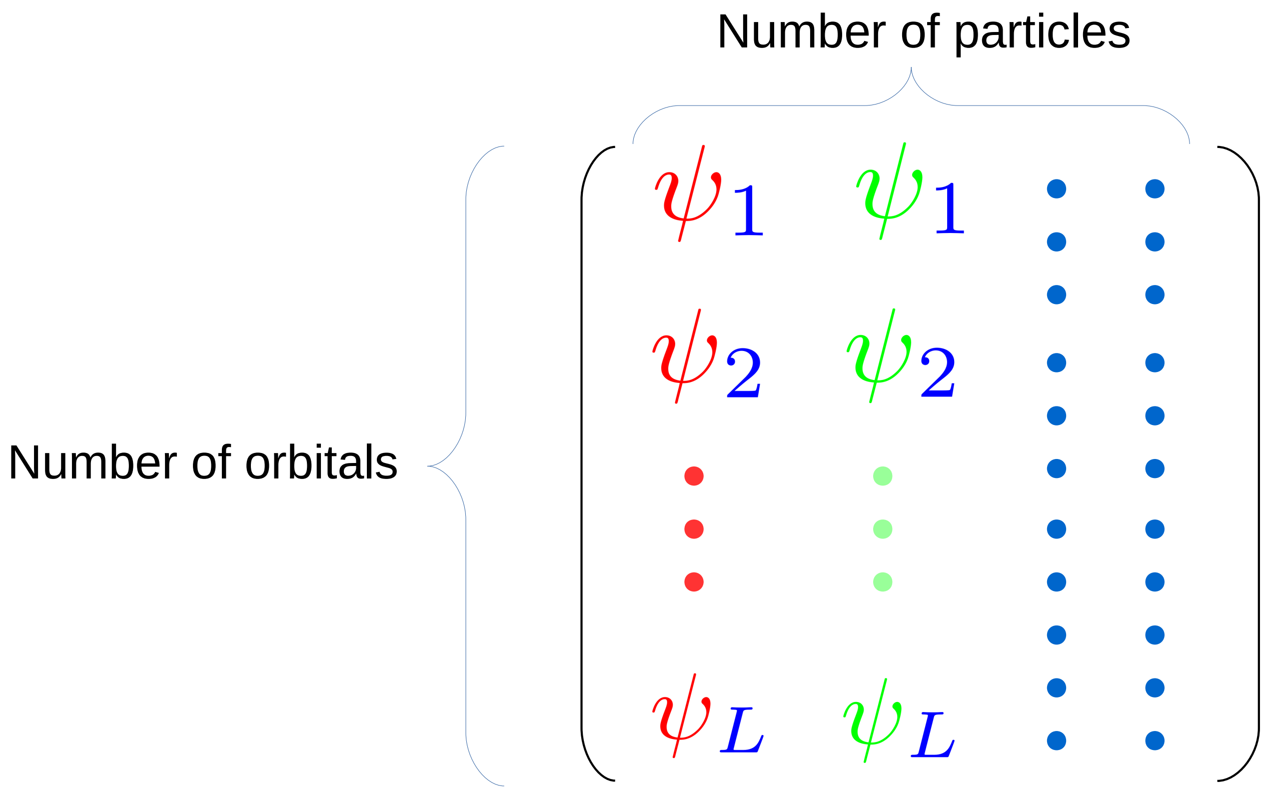

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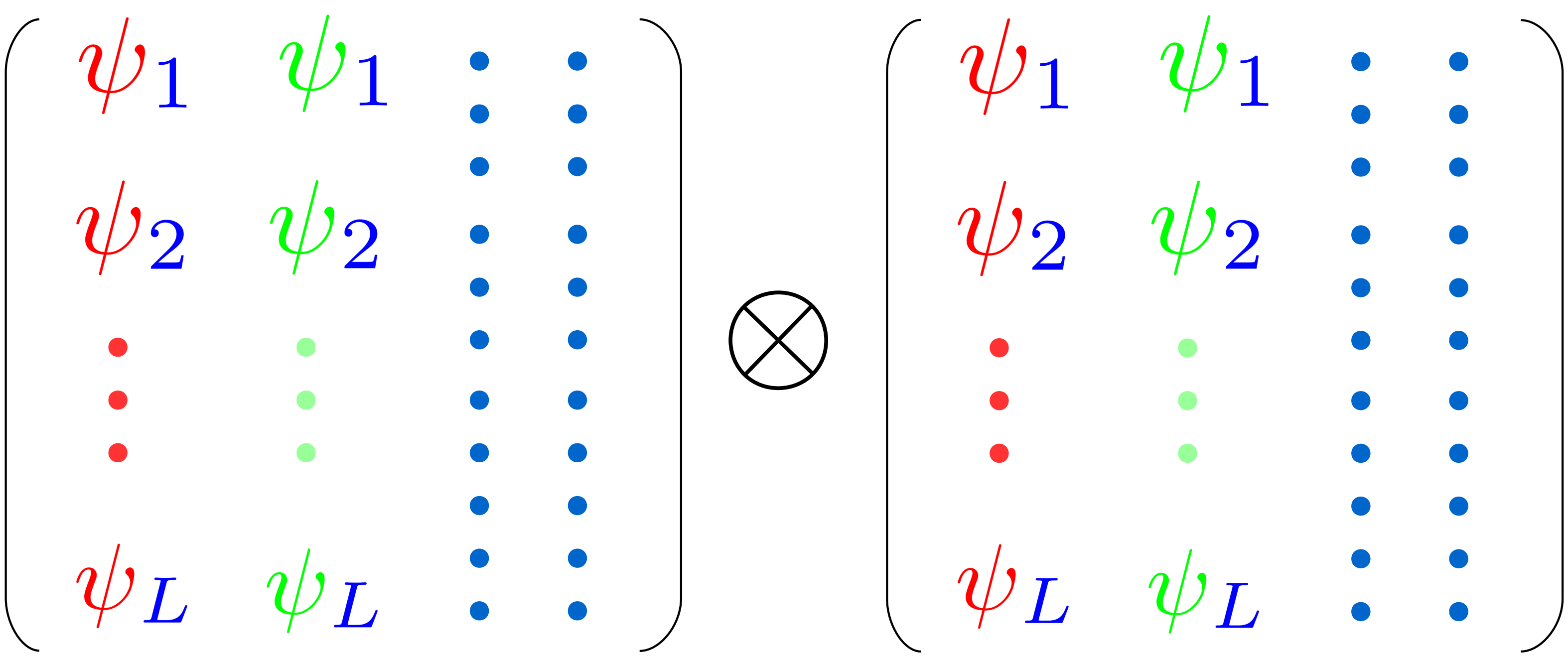

up-spin **down-spin**

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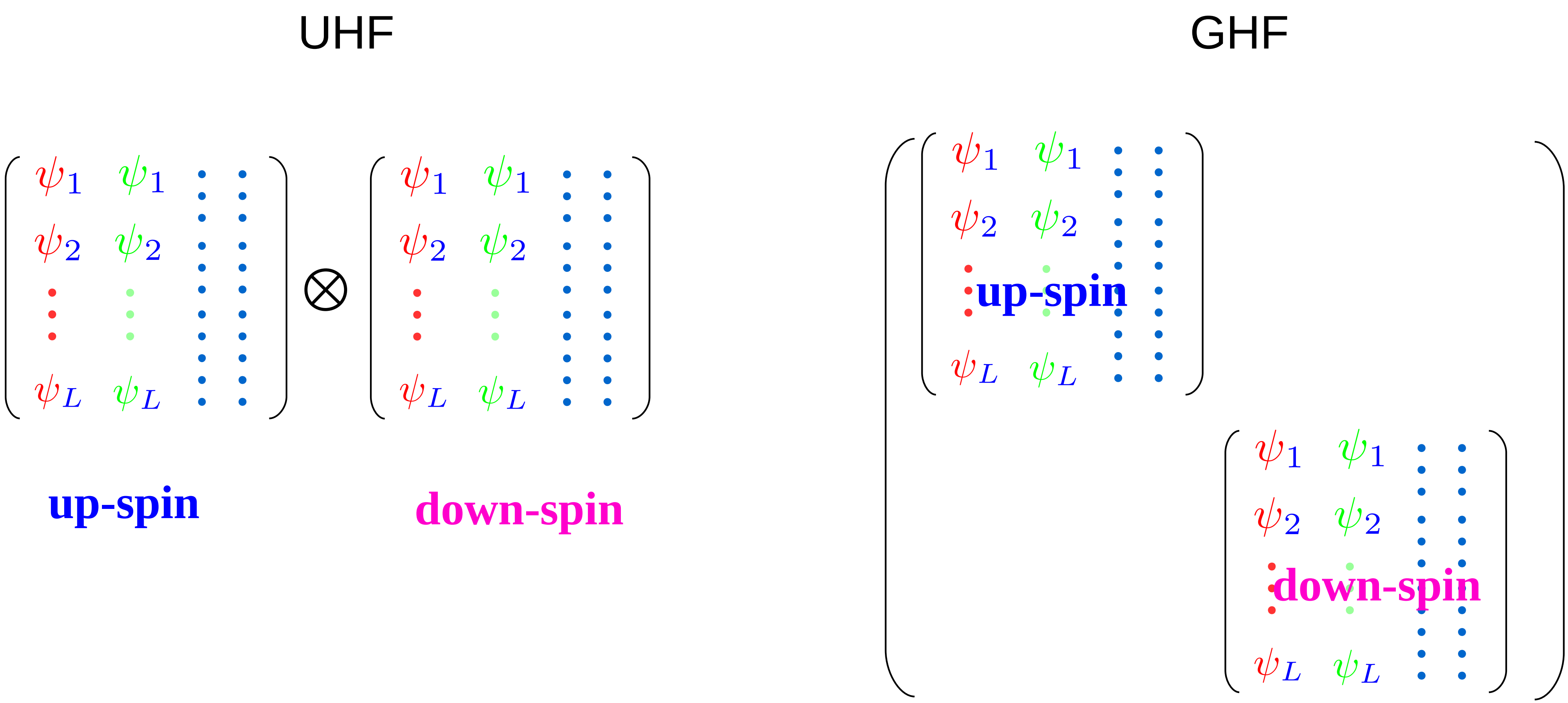

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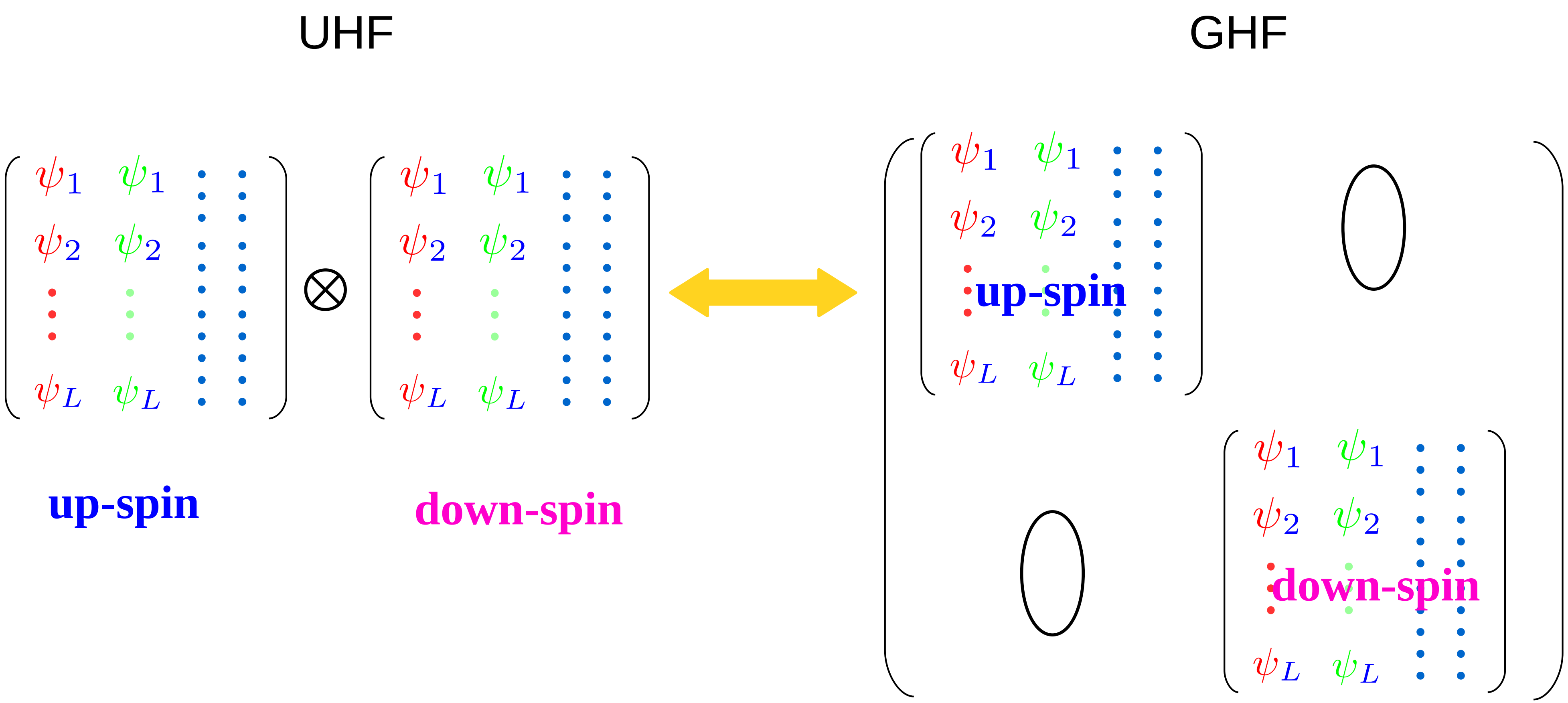

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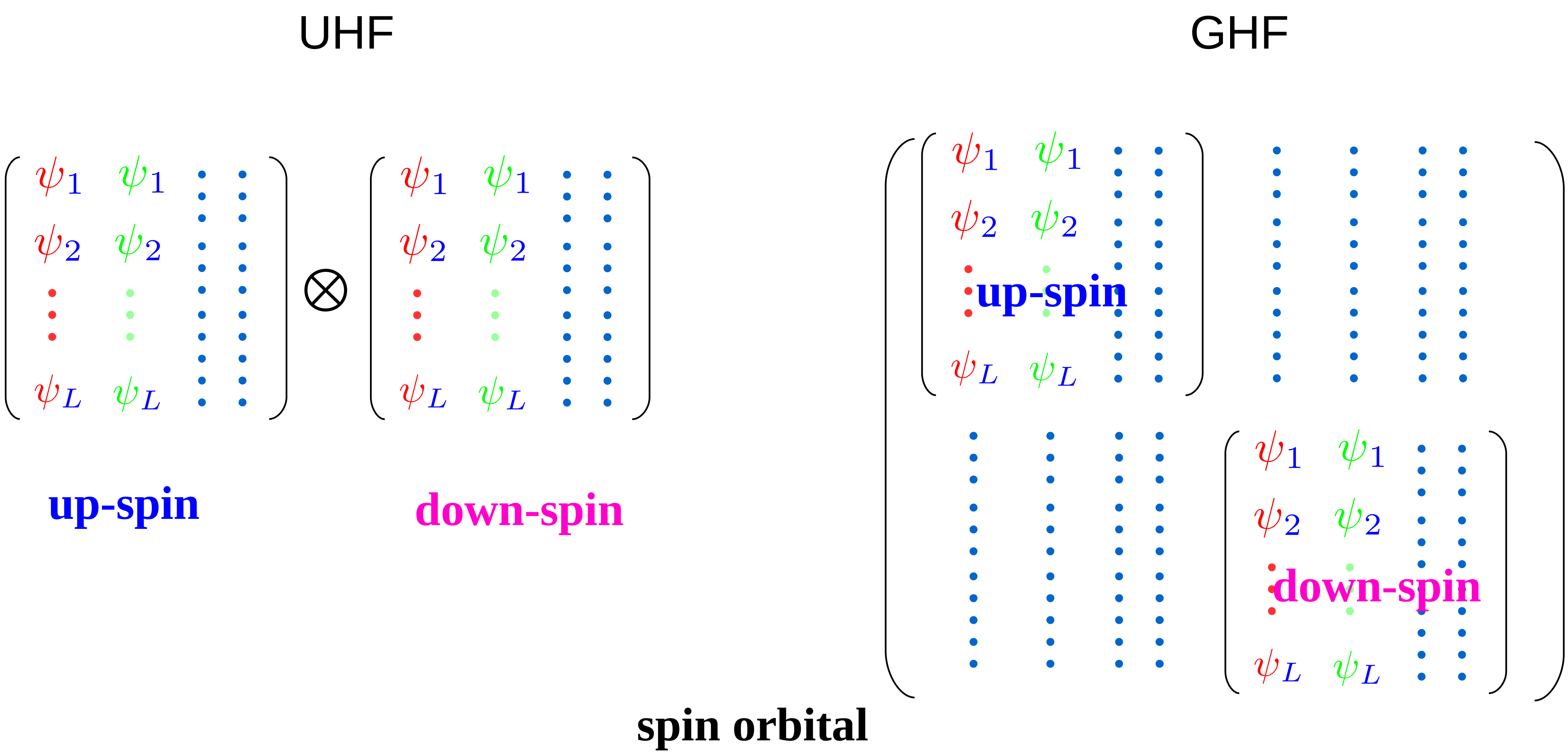

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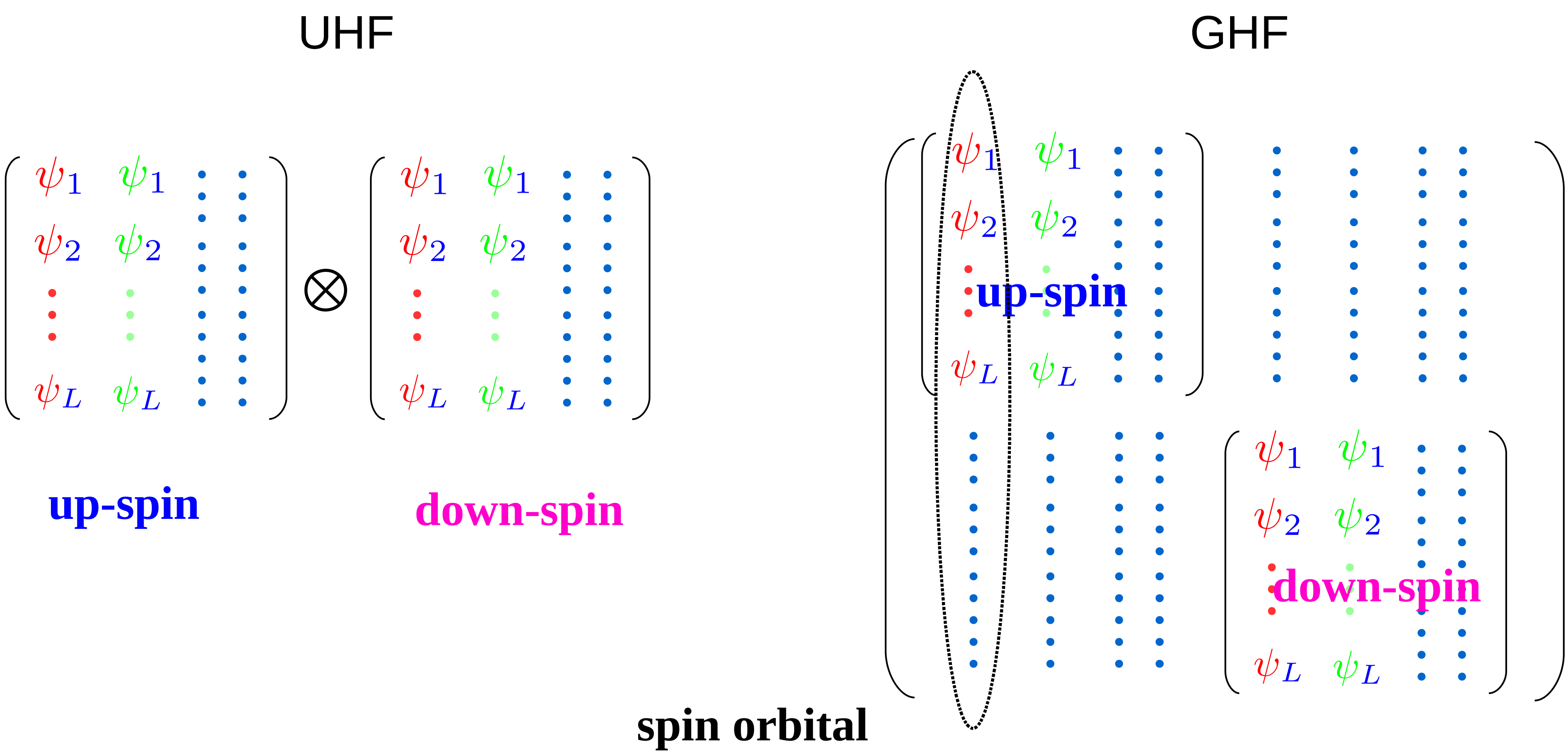

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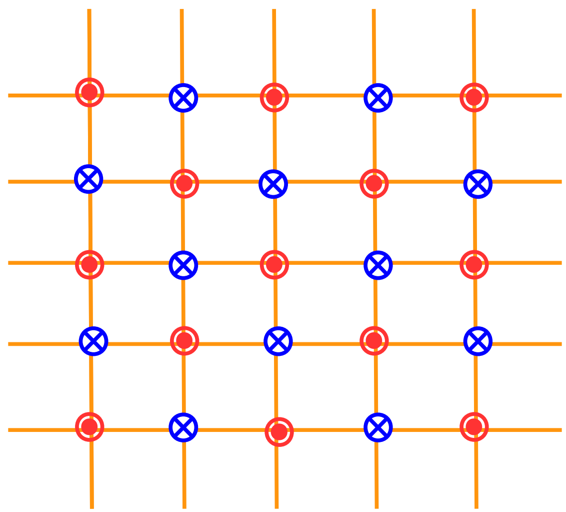
Generalized HF Trial Wave Function

- 2D repulsive Hubbard model: AFM order at Half-filling.

Trial wave function?

⊙ + z direction

⊗ - z direction



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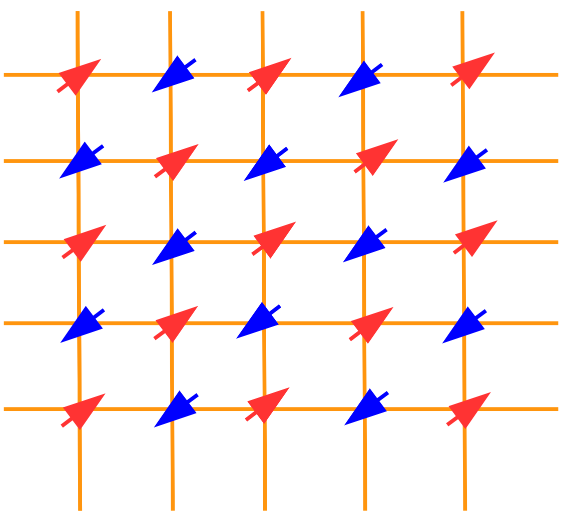

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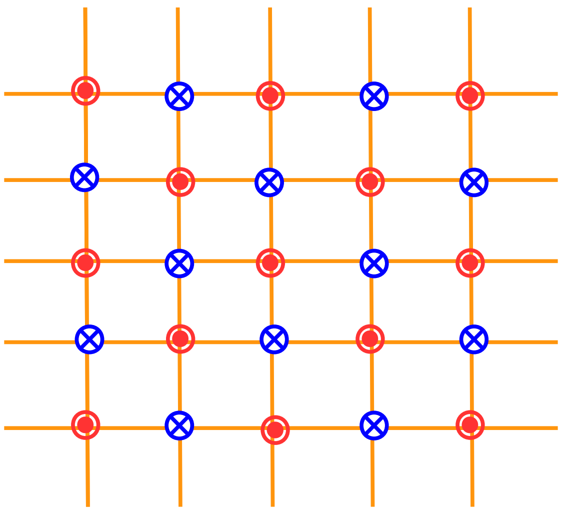

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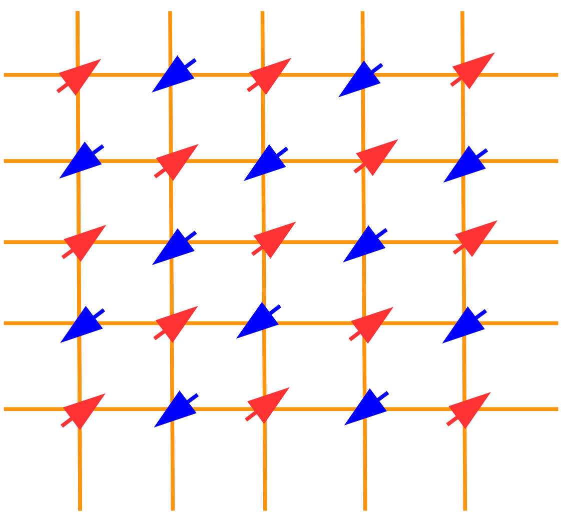

UHF

Break symmetry in z direction.
Preserve symmetry in xy direction.

GHF

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Preserve symmetry in z direction.

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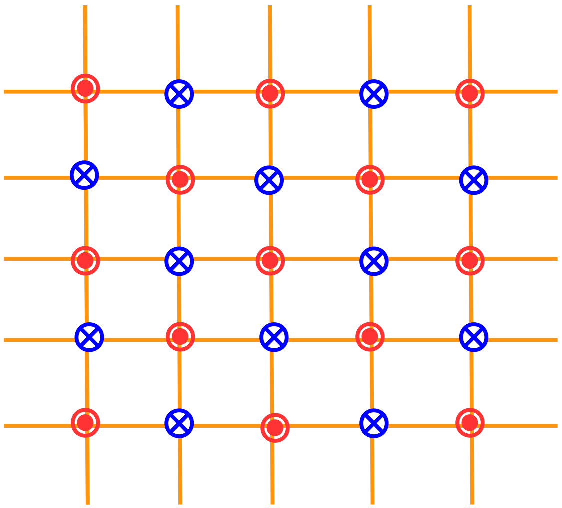

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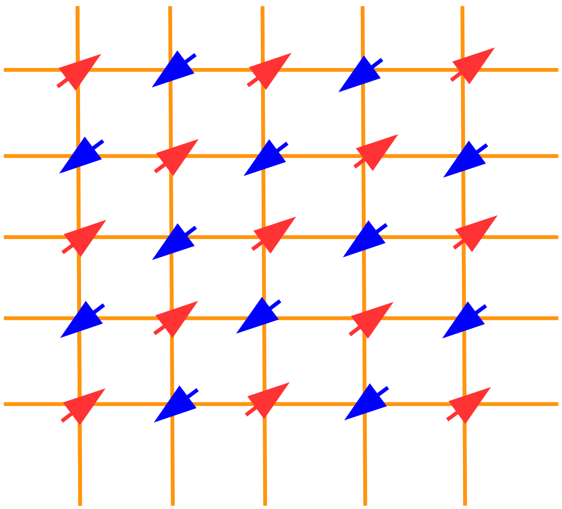

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UHF walker

Preserve symmetry in xy direction.

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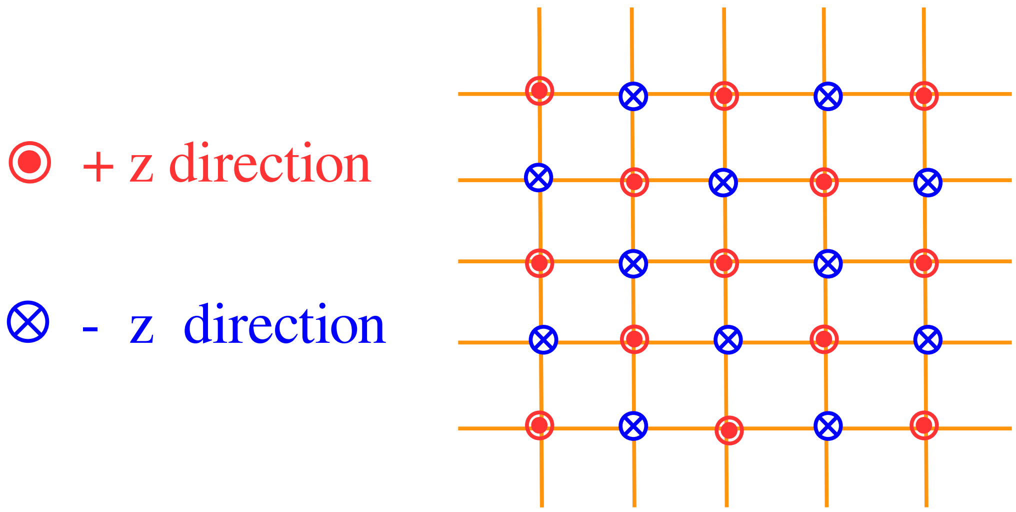

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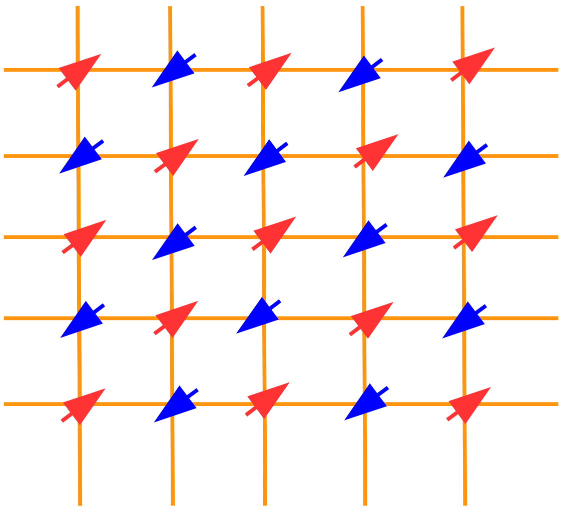

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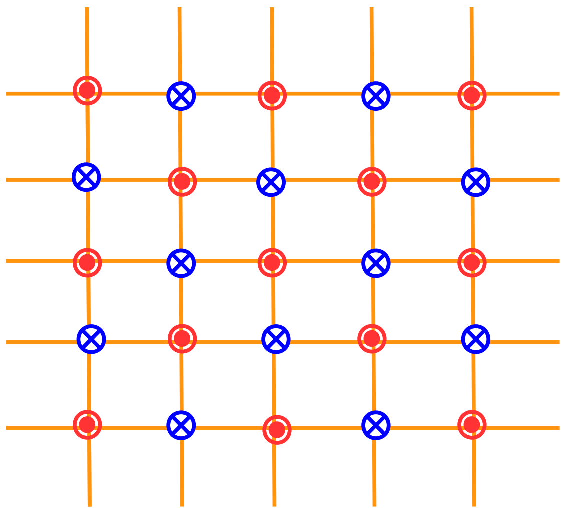

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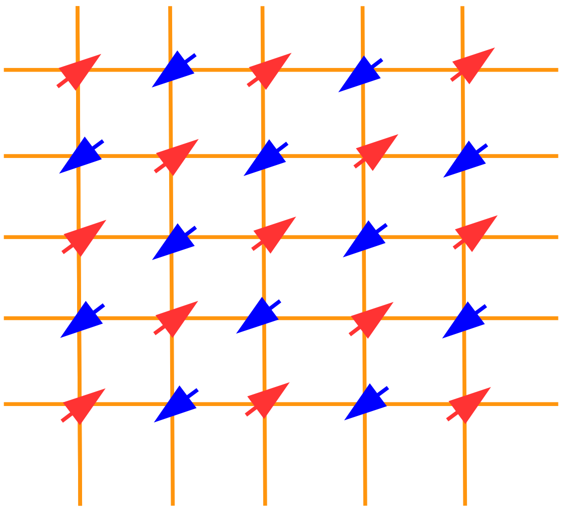

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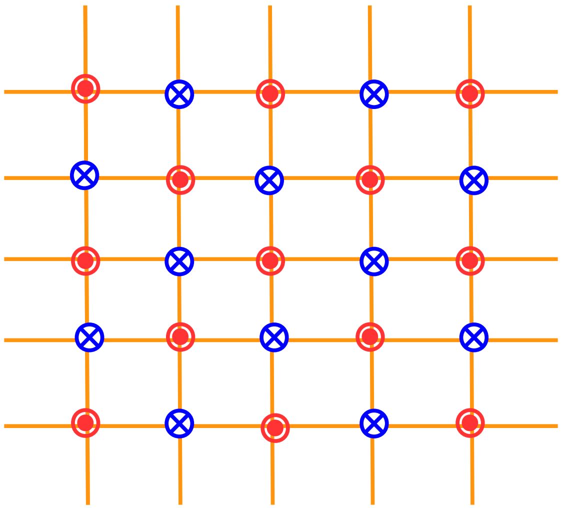

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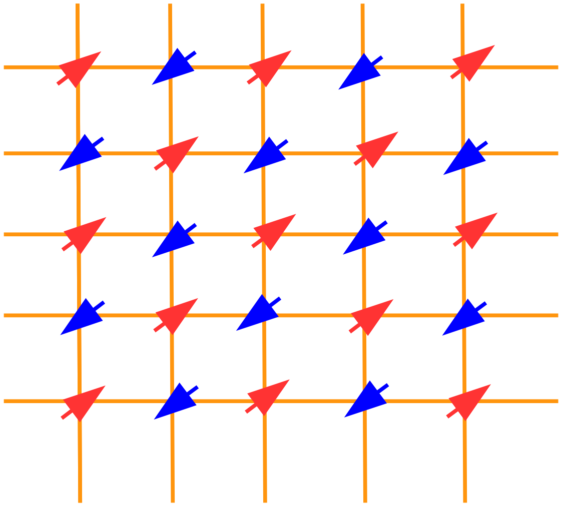

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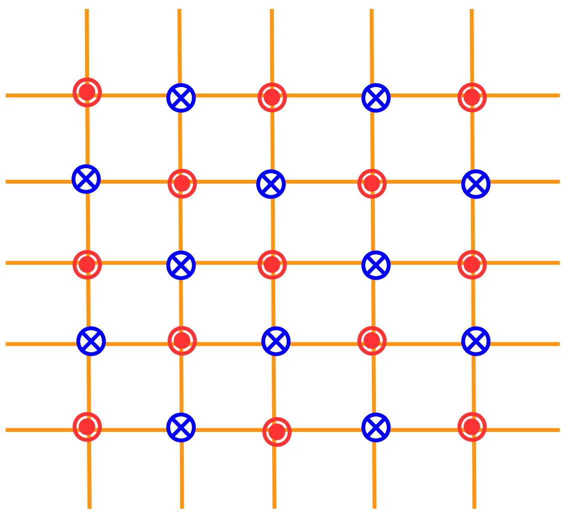

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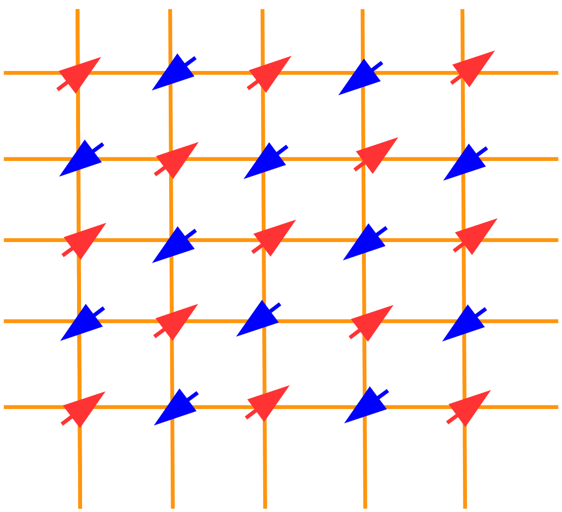


UHF

Break symmetry in z direction.
Preserve symmetry in xy direction.

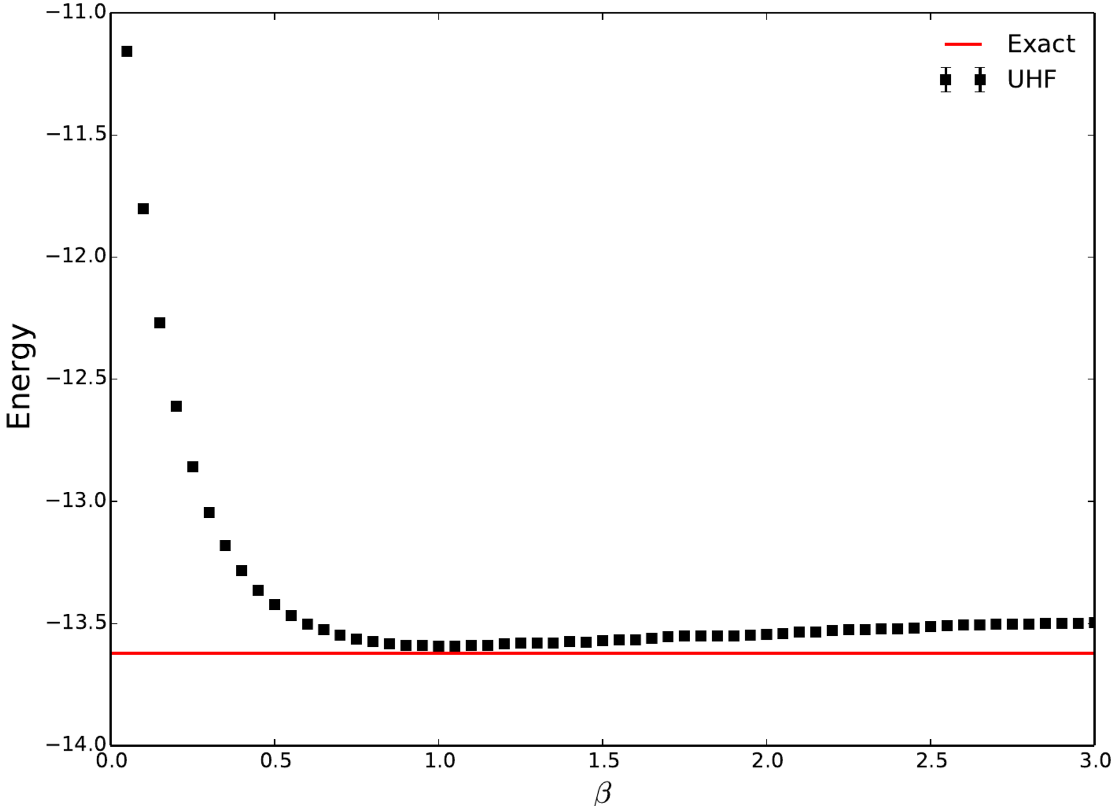
GHF

Preserve symmetry in all directions.

Generalized HF Trial Wave Function

- Half-filling Hubbard model:

  - no sign problem
  - add constraint deliberately
  - largest constraint bias



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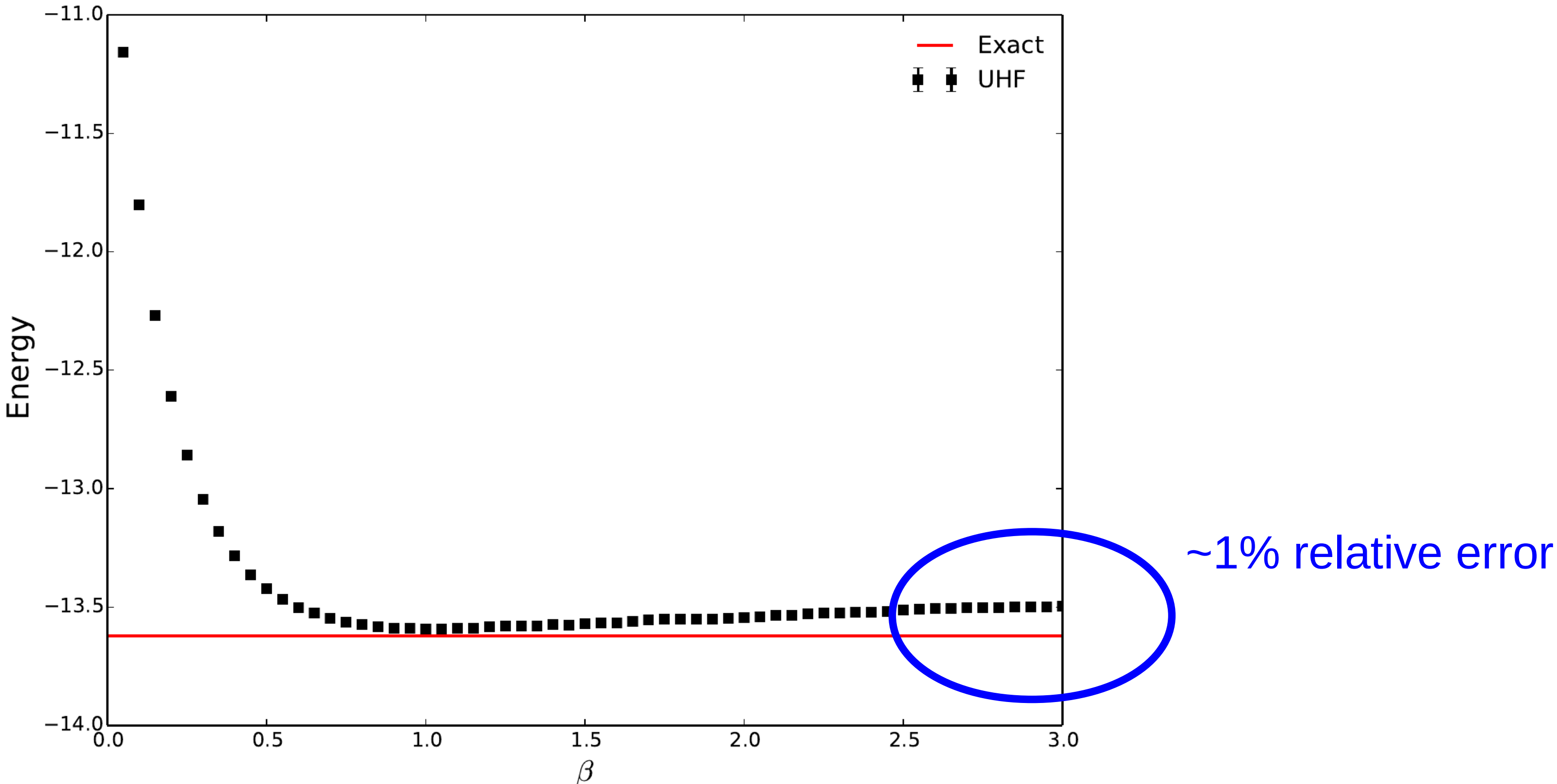

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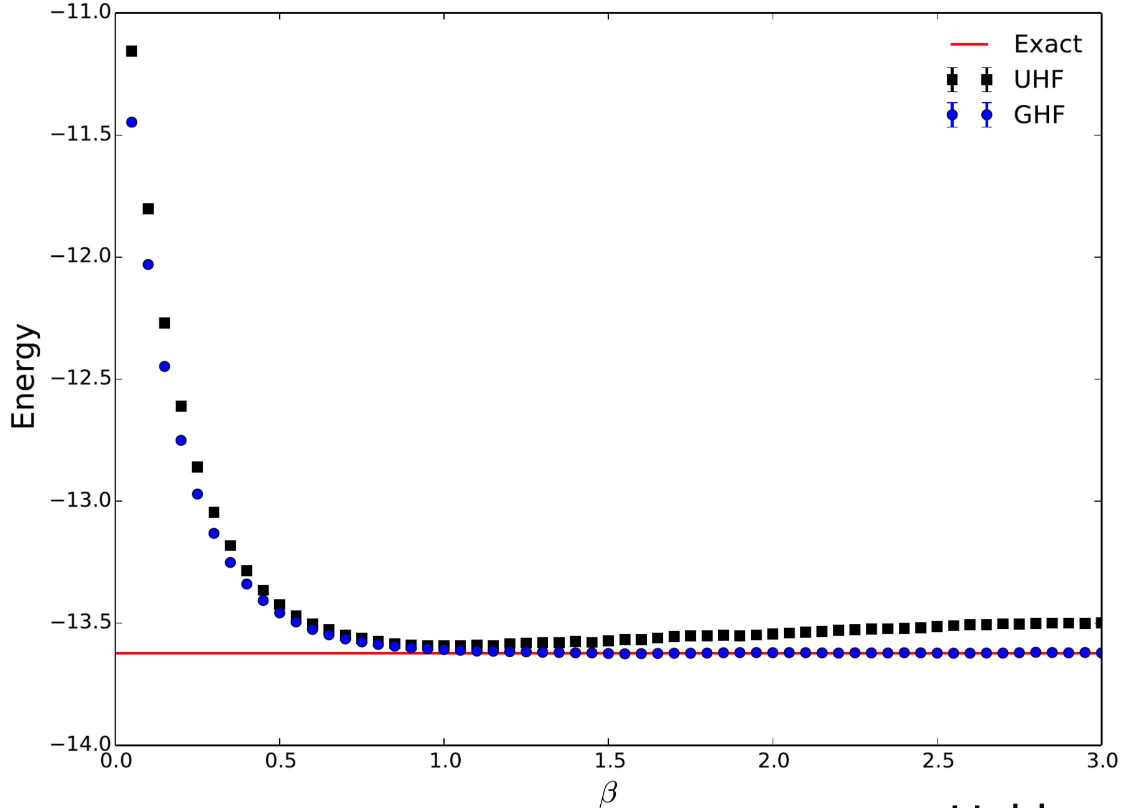

With GHF trial wave function, the result becomes exact!

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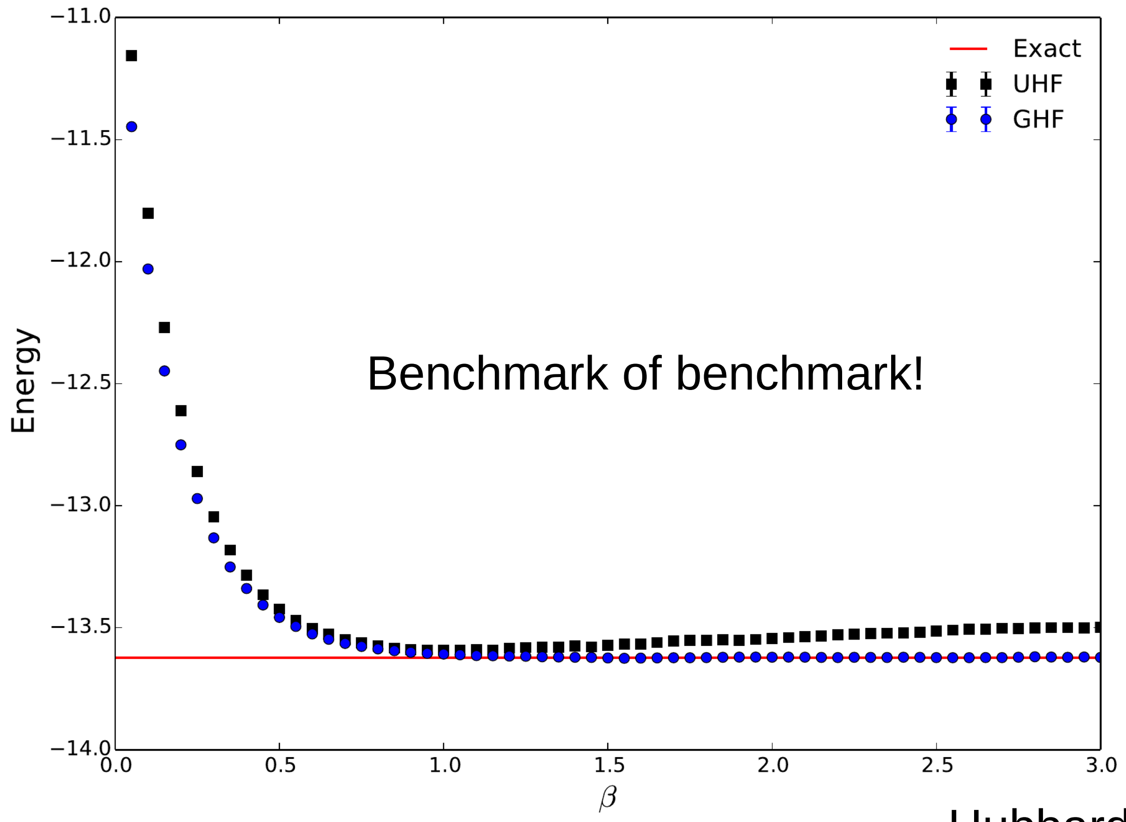

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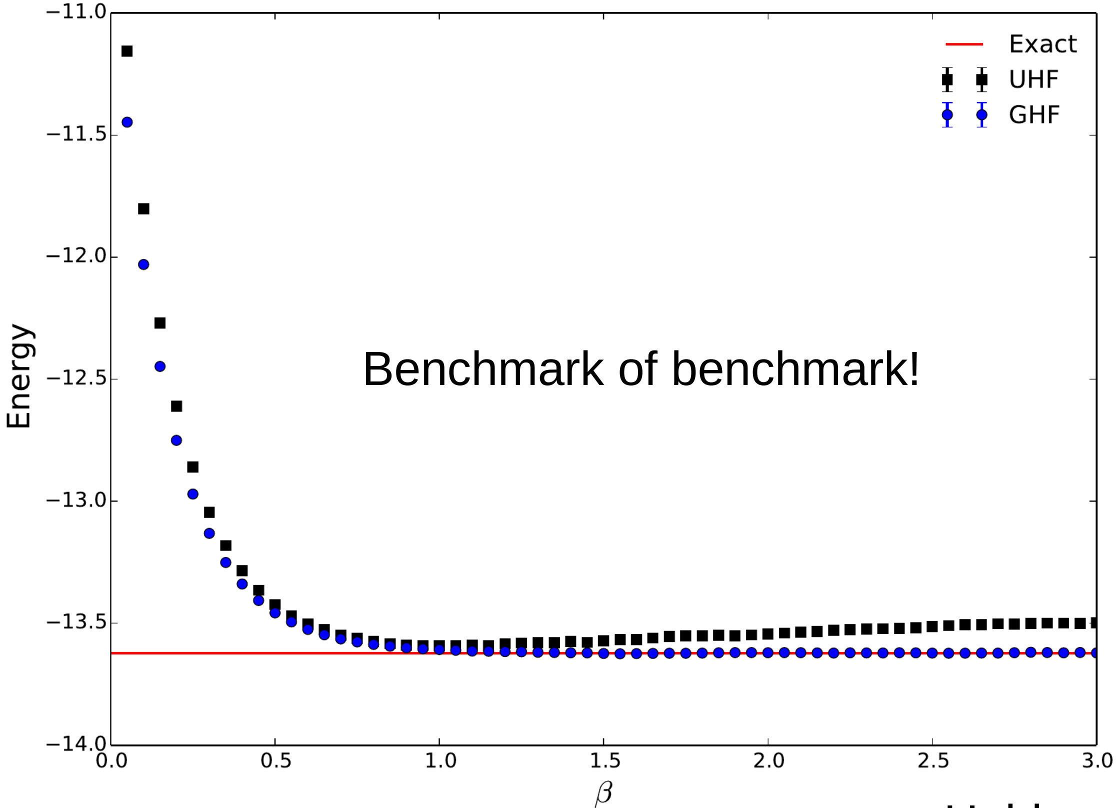
More benchmark results:
Emanuel Gull's talk!



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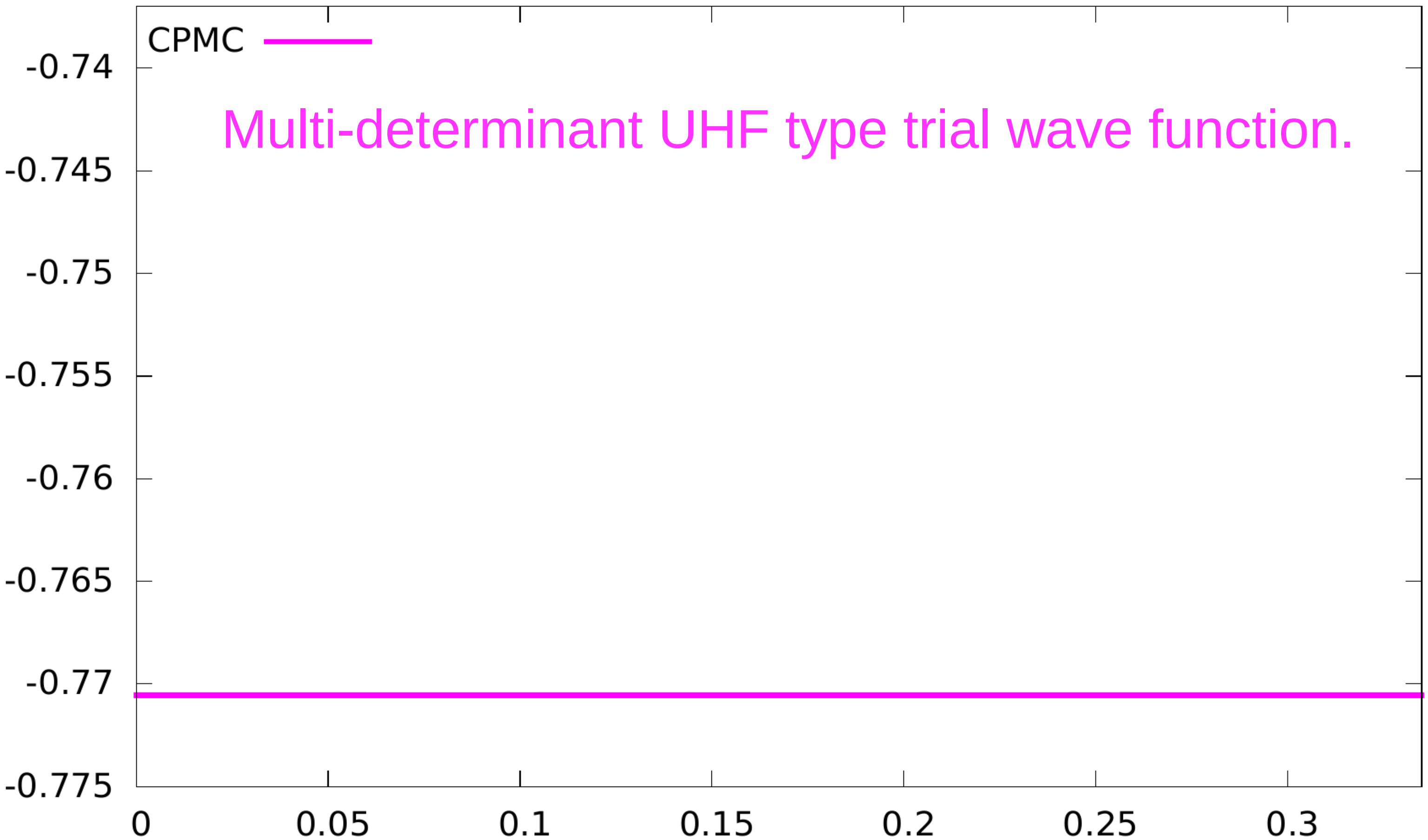
Doped Hubbard Model

- 16x4 ladder, 1/8 doping, U=8



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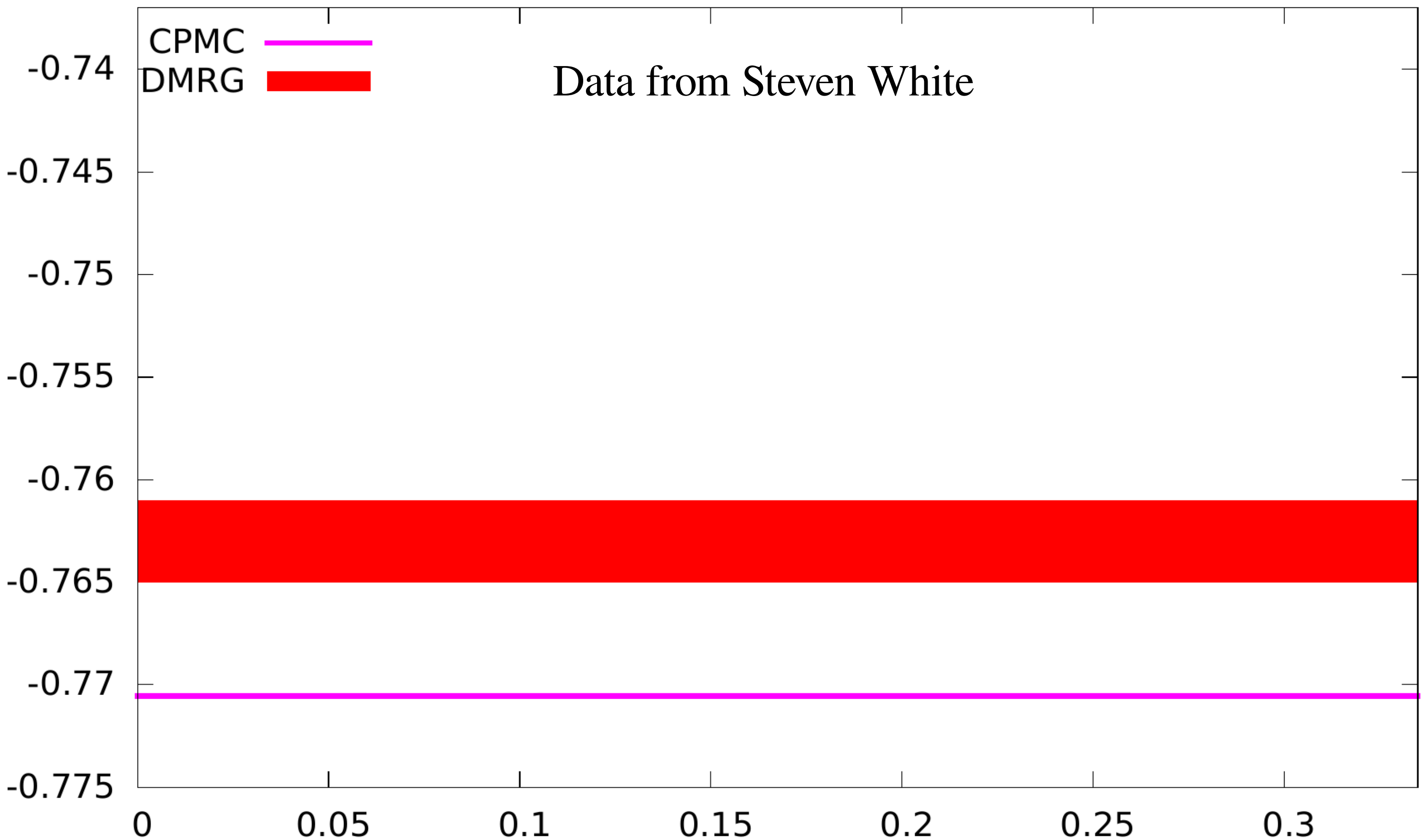

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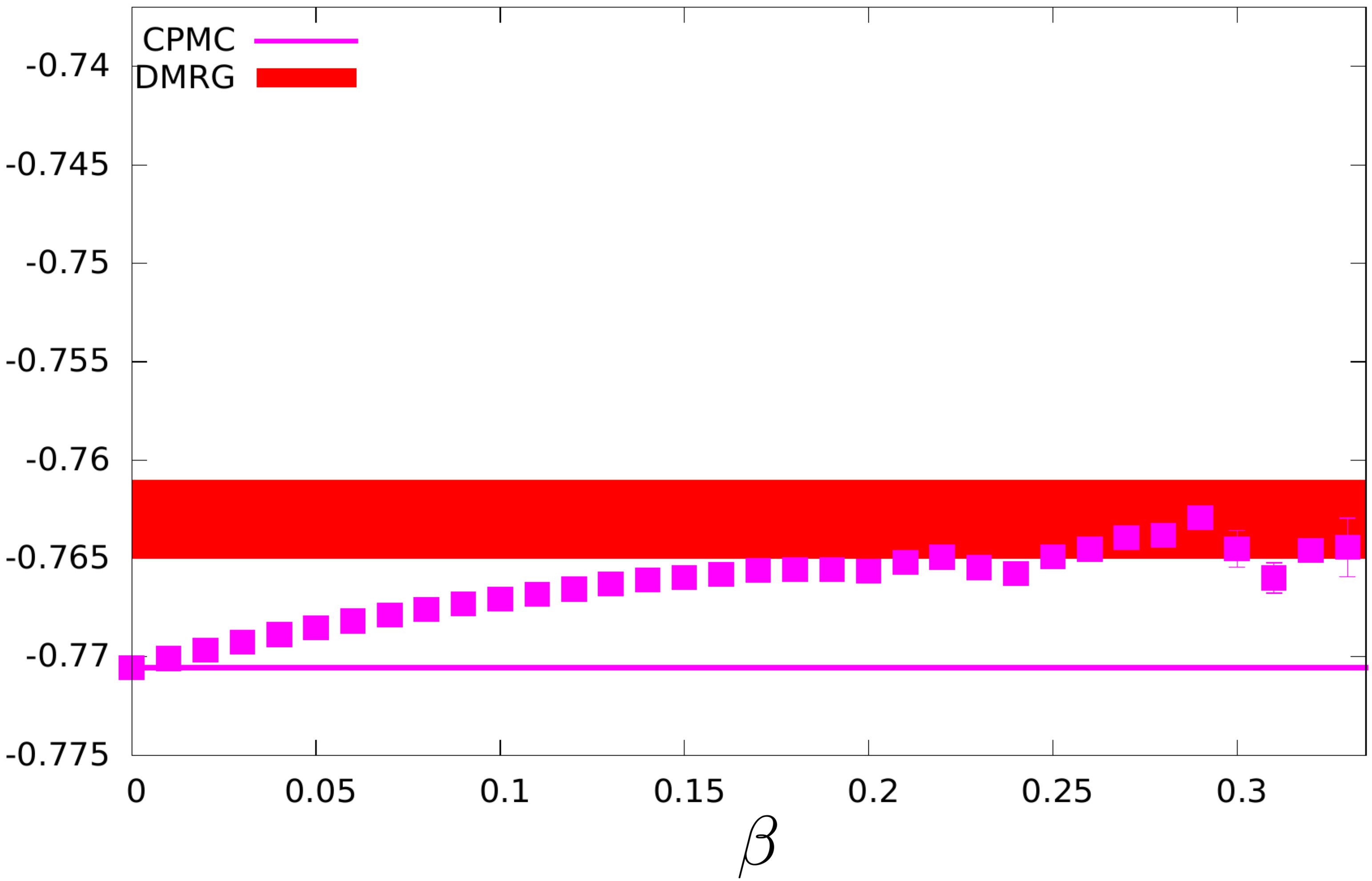

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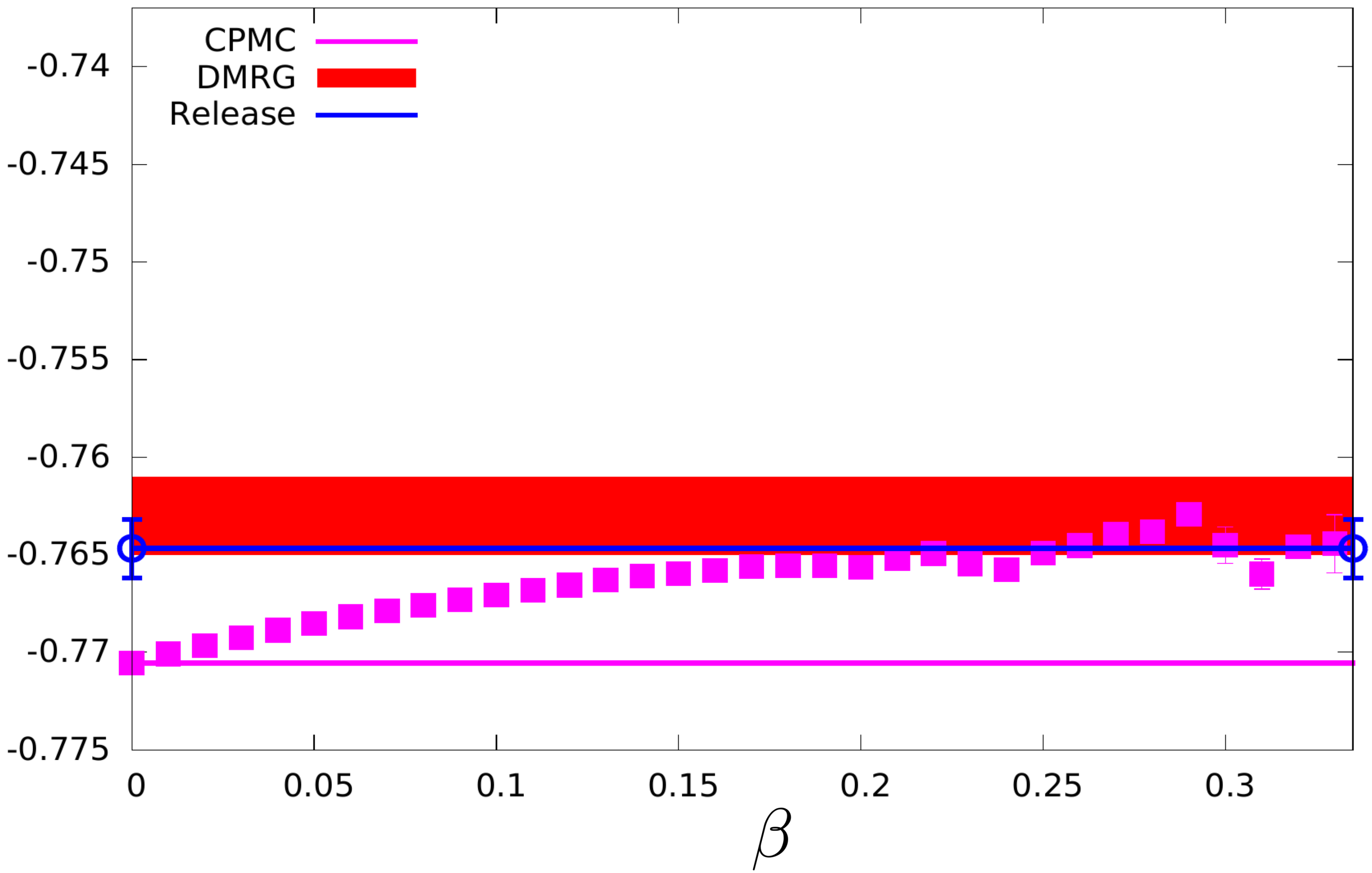

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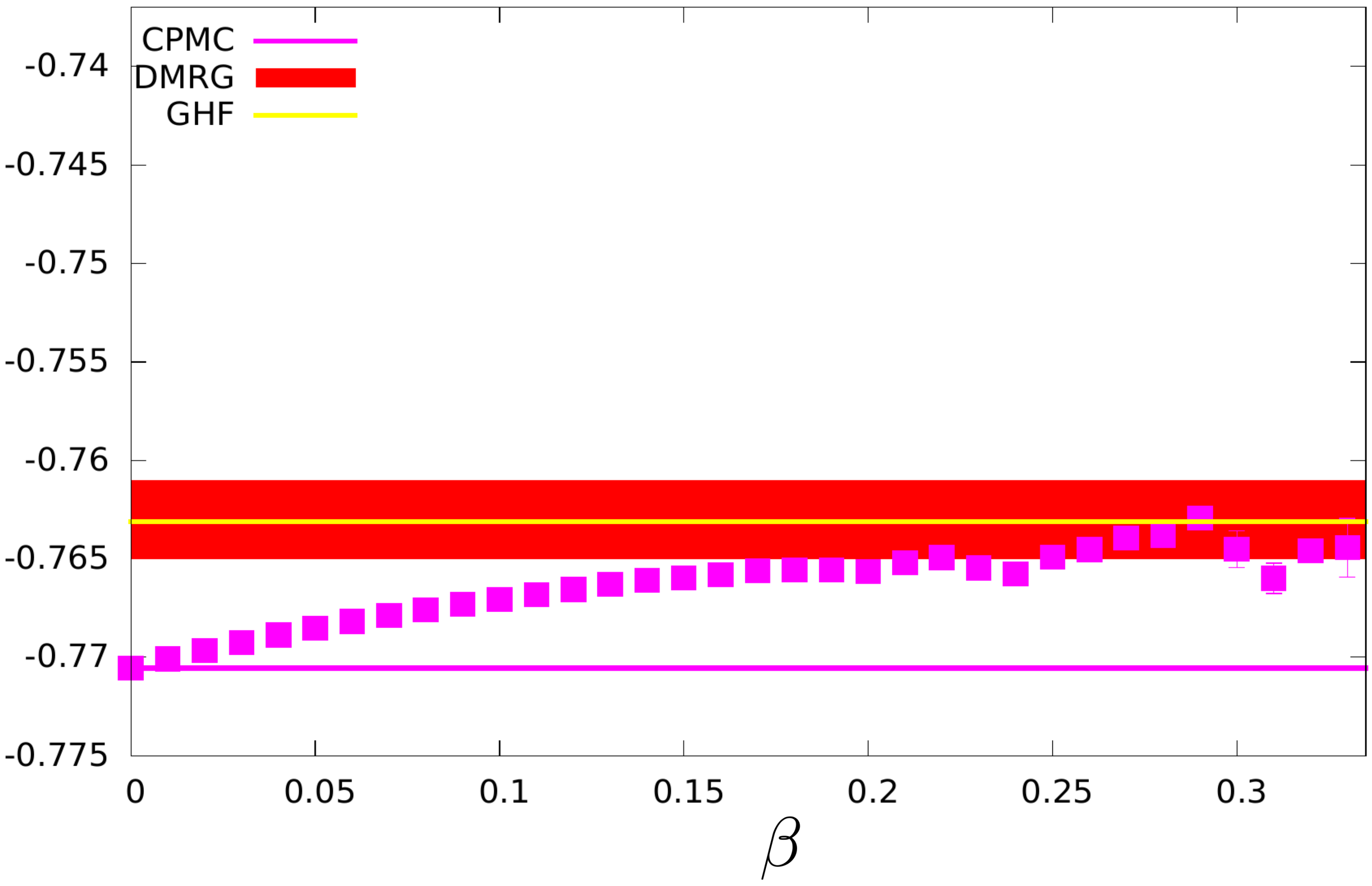

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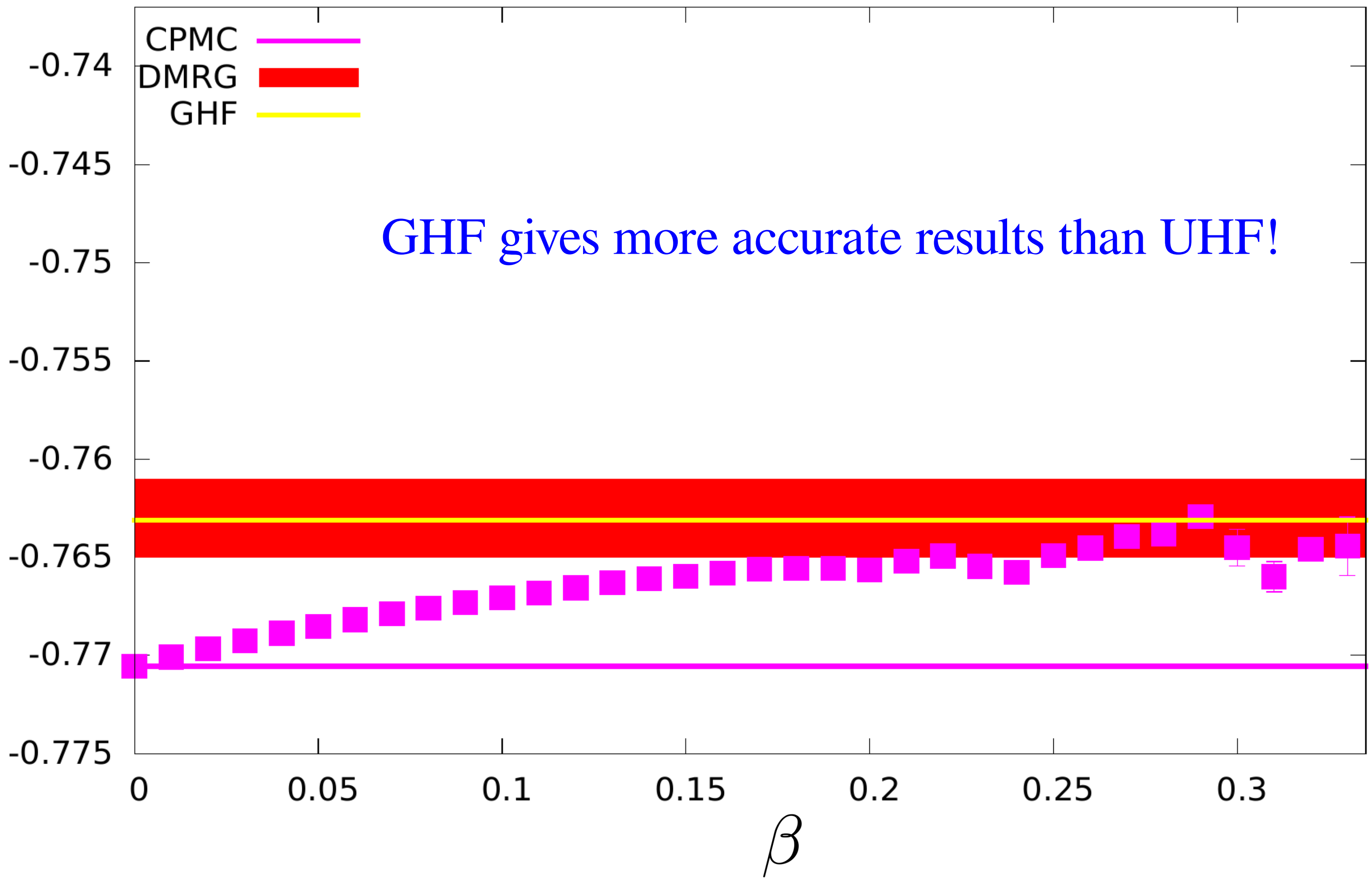

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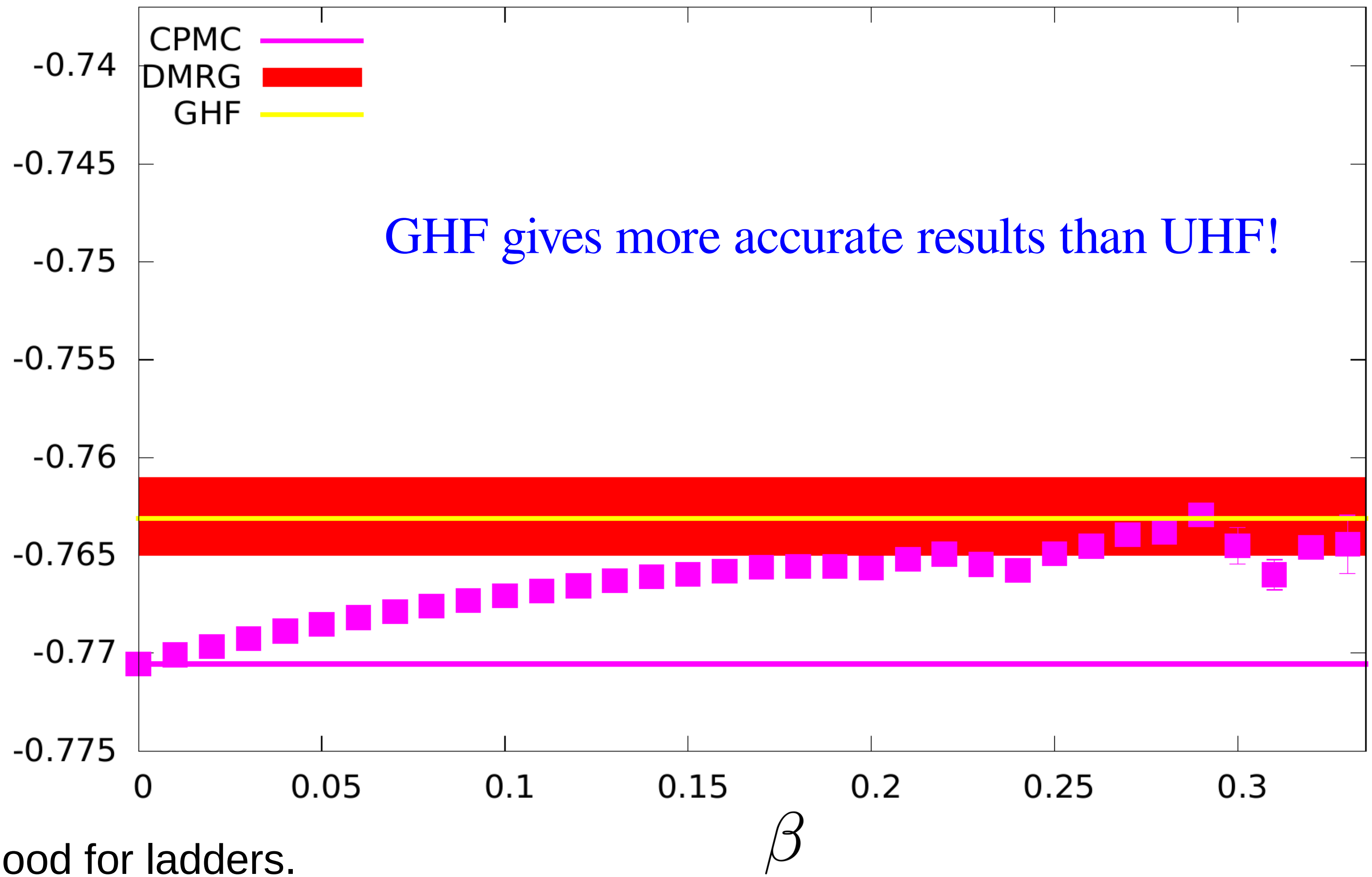


DMRG is good for ladders.

Doped Hubbard Model

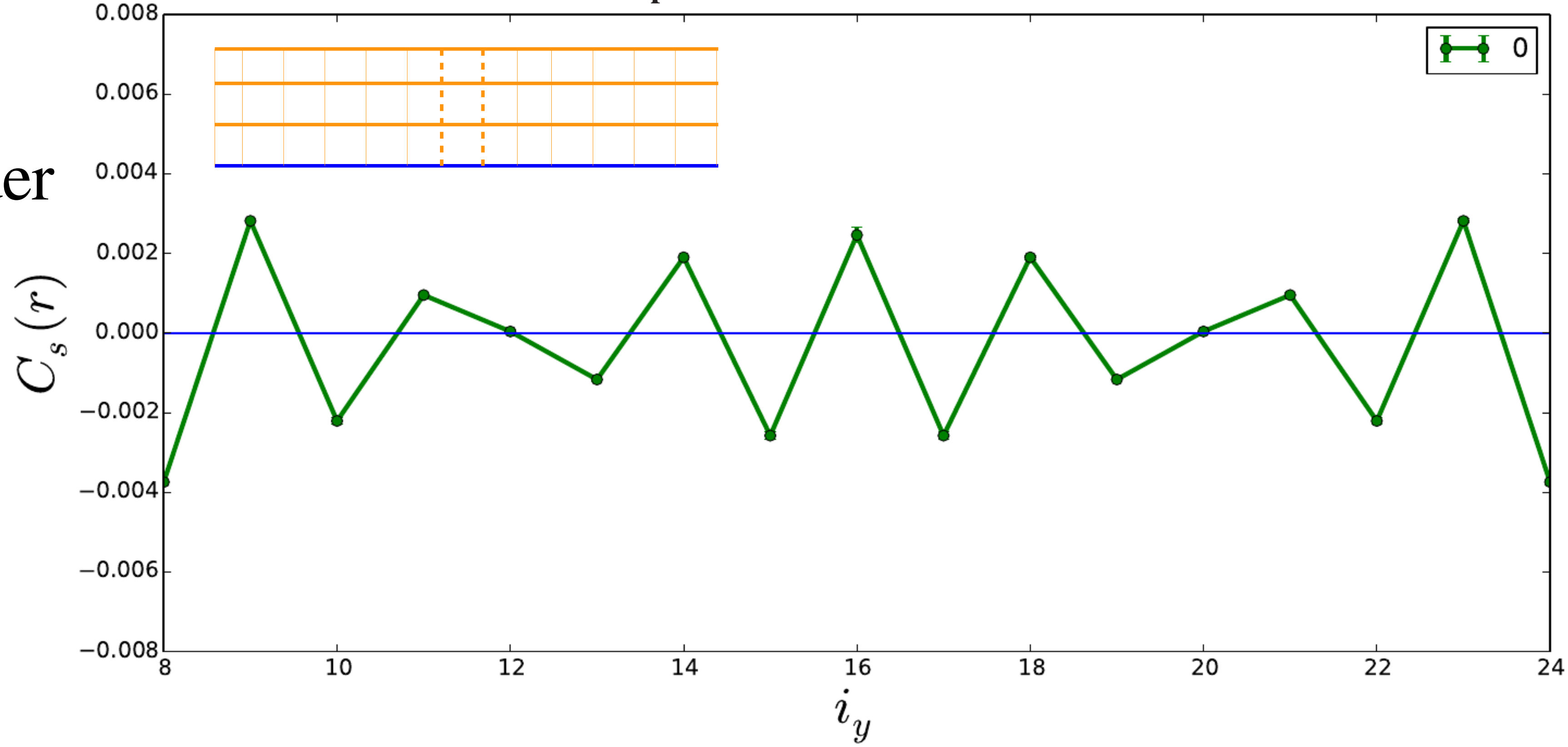
- GHF trial wave function

$$C_s(\mathbf{r}) = \frac{1}{N}\sum_{\mathbf{r}'}\langle(n_{\mathbf{r}+\mathbf{r}',\uparrow} - n_{\mathbf{r}+\mathbf{r}',\downarrow})(n_{\mathbf{r}',\uparrow} - n_{\mathbf{r}',\downarrow})\rangle$$

32x4 ladder

h=1/8

U=4



Ongoing!

Doped Hubbard Model

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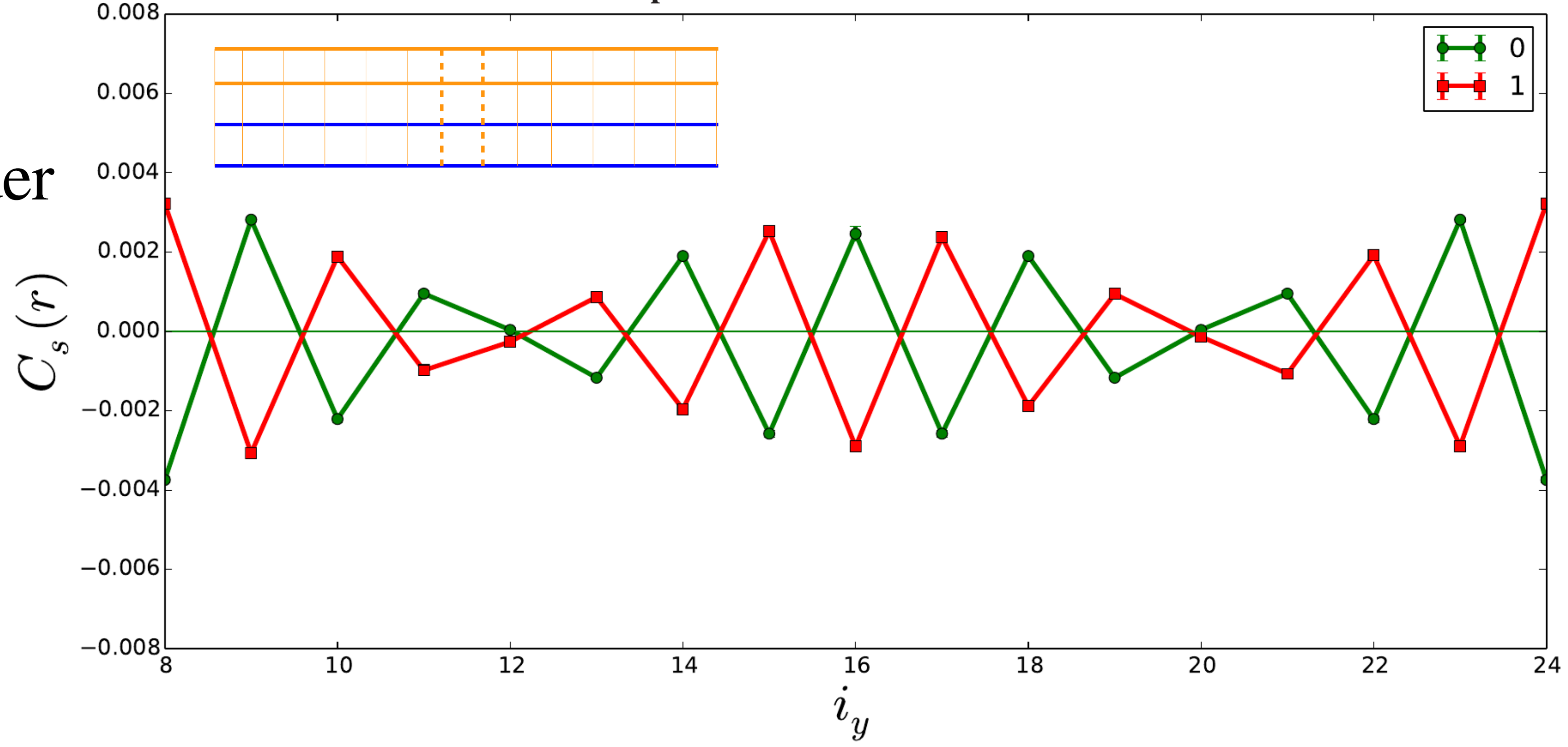

Ongoing!

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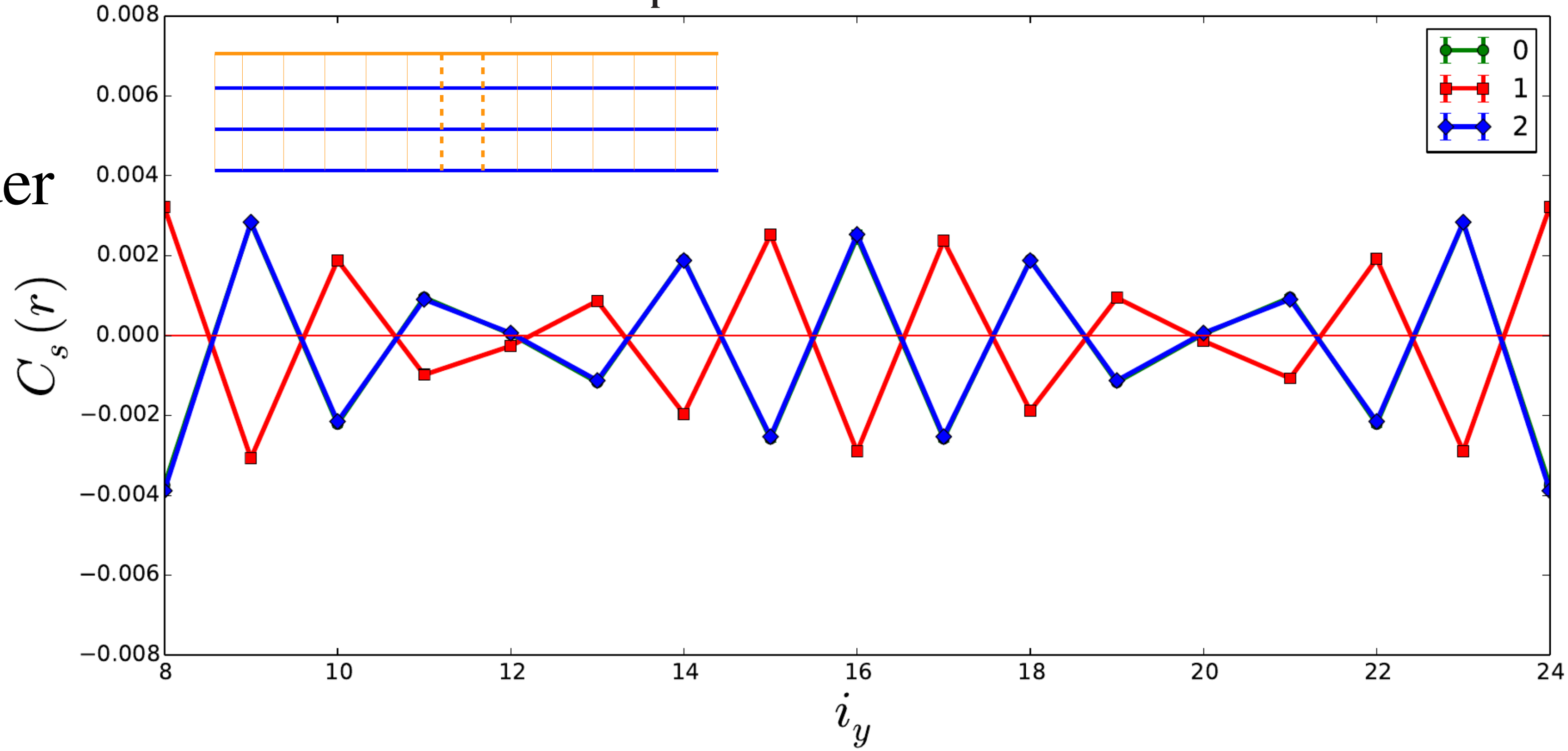

Ongoing!

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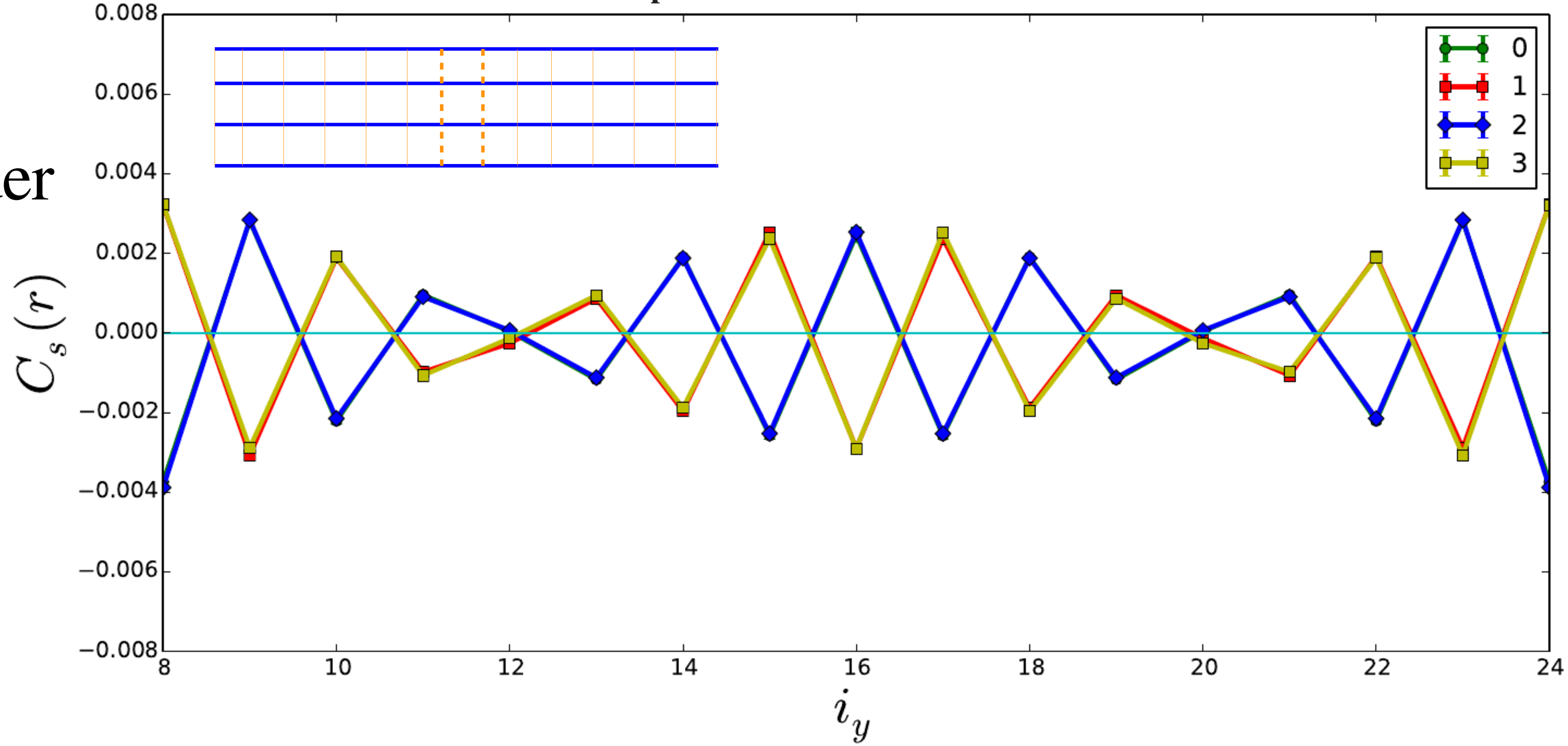

Ongoing!

Doped Hubbard Model

- GHF trial wave function

$$C'_s(l_x, l_y) \equiv (-1)^{l_y} C_s(l_x, l_y)$$

32x4 ladder

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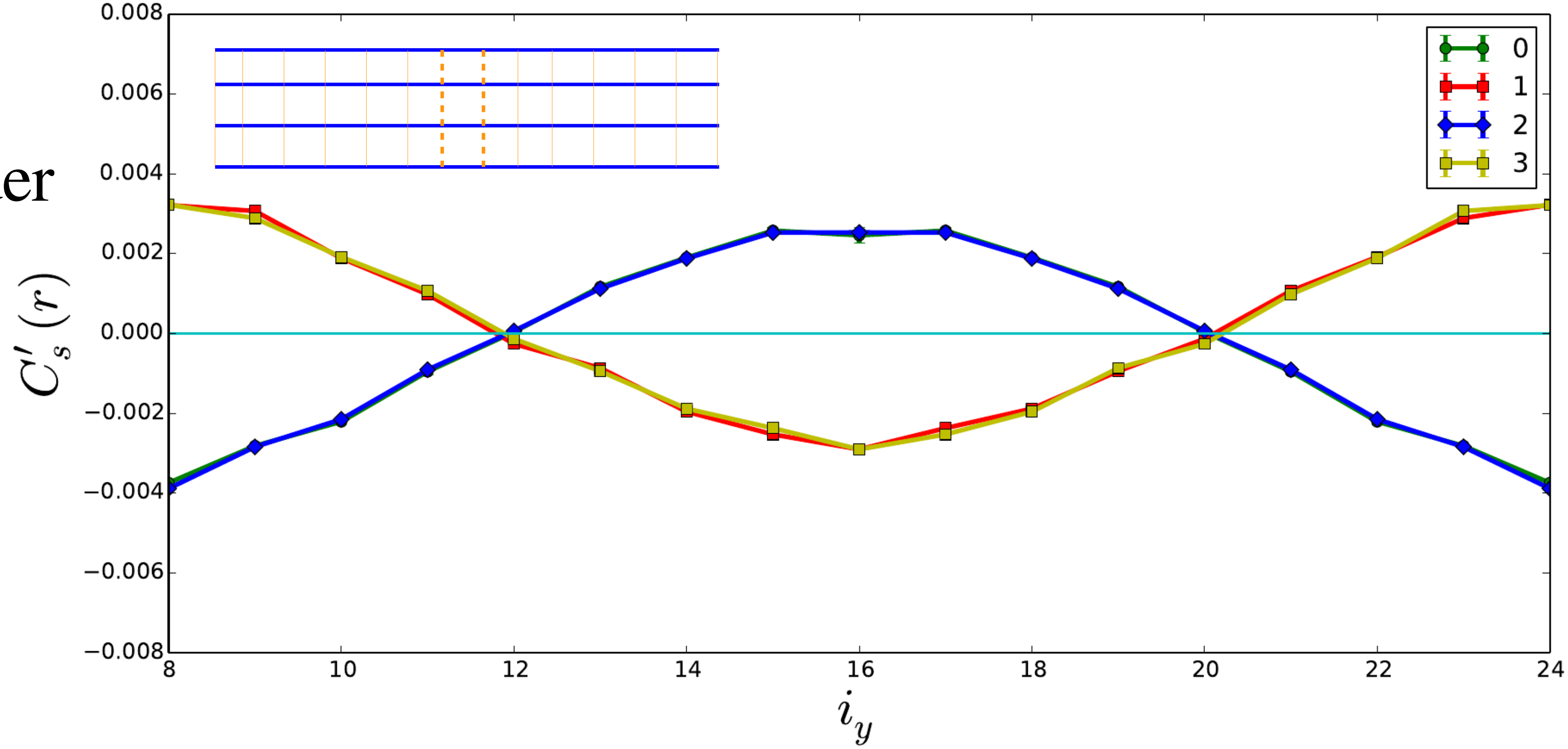

Ongoing!

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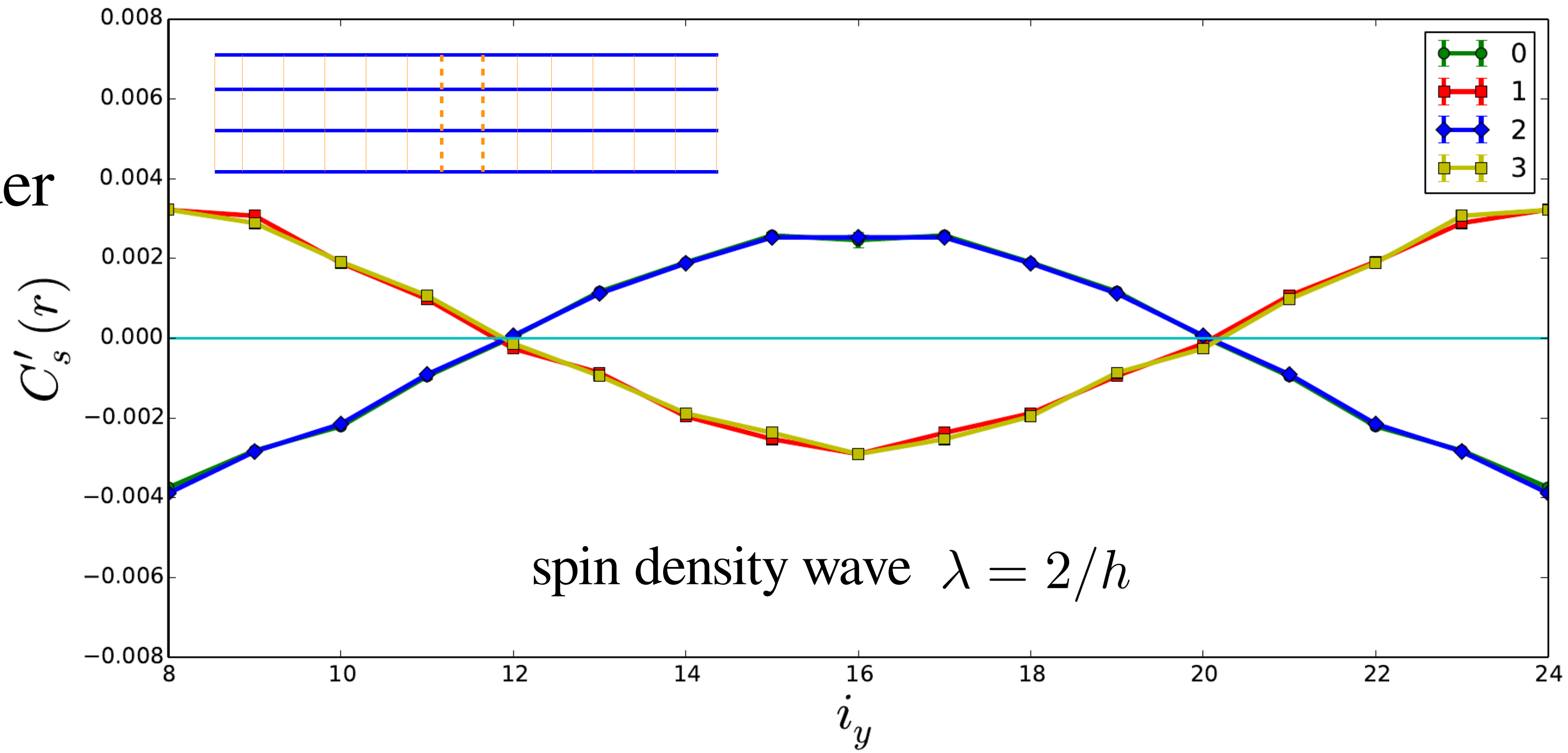

Consistent with earlier results using free-electron trial wfs: Chang & Zhang, PRL (2010)

Ongoing!

Outline

- Introduction to AFQMC
  - Release constraint
  - Symmetry in trial wave function
  - Generalized Hartree–Fock (GHF) wave function
- Magnetic orders in 2D Hubbard model — GHF trial wave function
  - Half-filling: restores symmetry
  - Doped: more accurate results
- **Rashba spin-orbit coupling in 2D Fermi gas** — GHF random walker
  - Interplay between SOC and interaction
  - Singlet triplet pairing wave function
- Conclusion

2D Fermi Gas with Rashba Spin-orbit Coupling

$$H = \sum_{\mathbf{k}\sigma} k^2 c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + \sum_{\mathbf{k}} \lambda (k_y - i k_x) c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + h.c.$$

For details on FG w/o SOC, see arXiv:1504.00925

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Rashba SOC: Couples spin to momentum with strength λ allows for spin flips.

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Sample GHF wave function in AFQMC!

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SOC and strong interaction in ultra-cold atom experiment.

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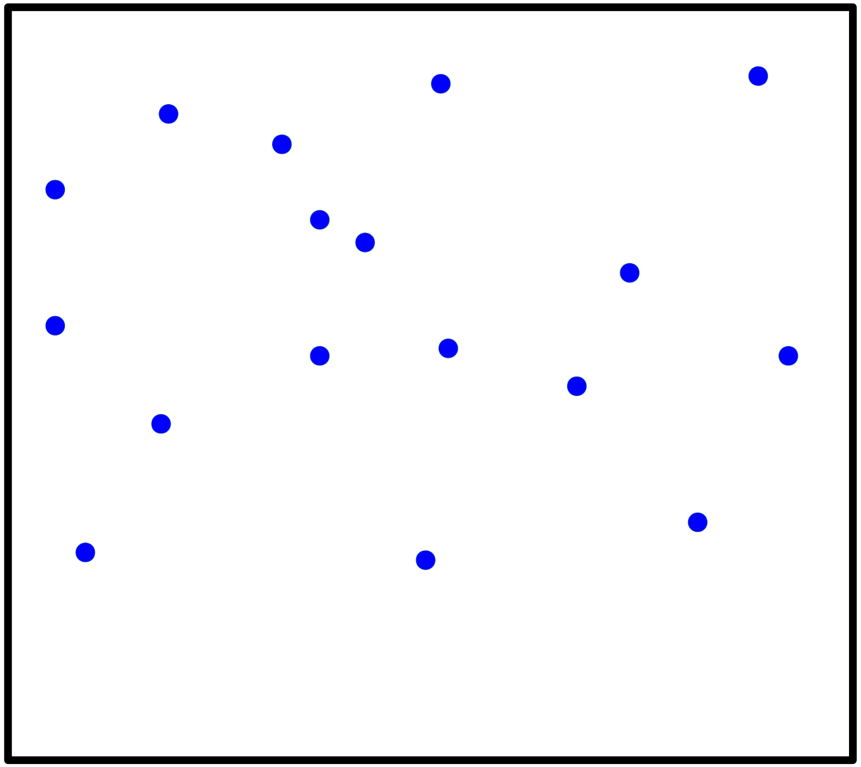

Particles in the box

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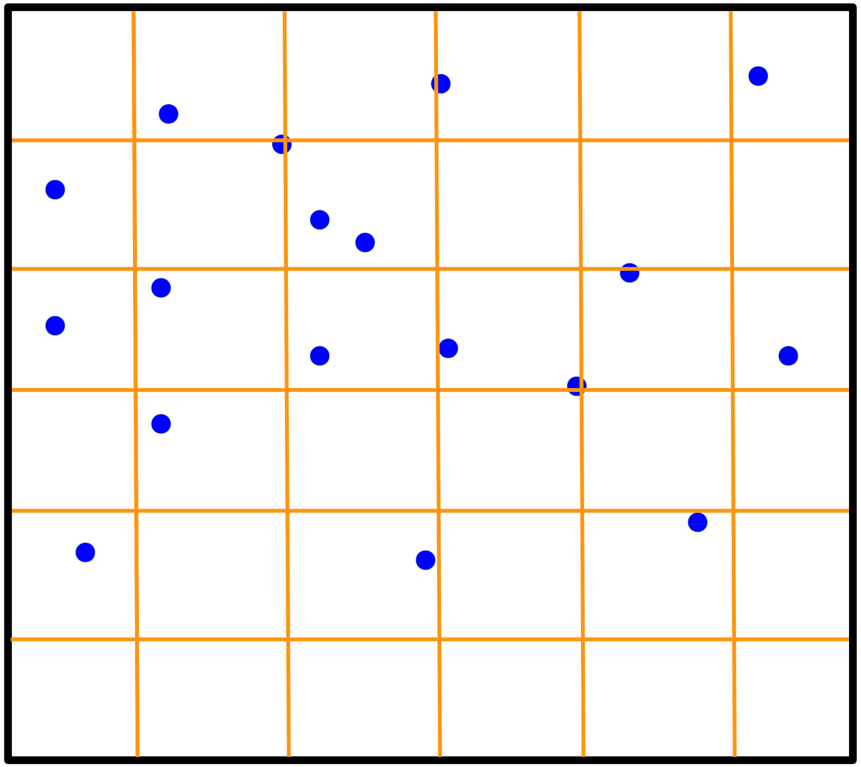
discretization!



Lattice size: L

Number of particles: N

$$n = N/L$$

Particles in the box

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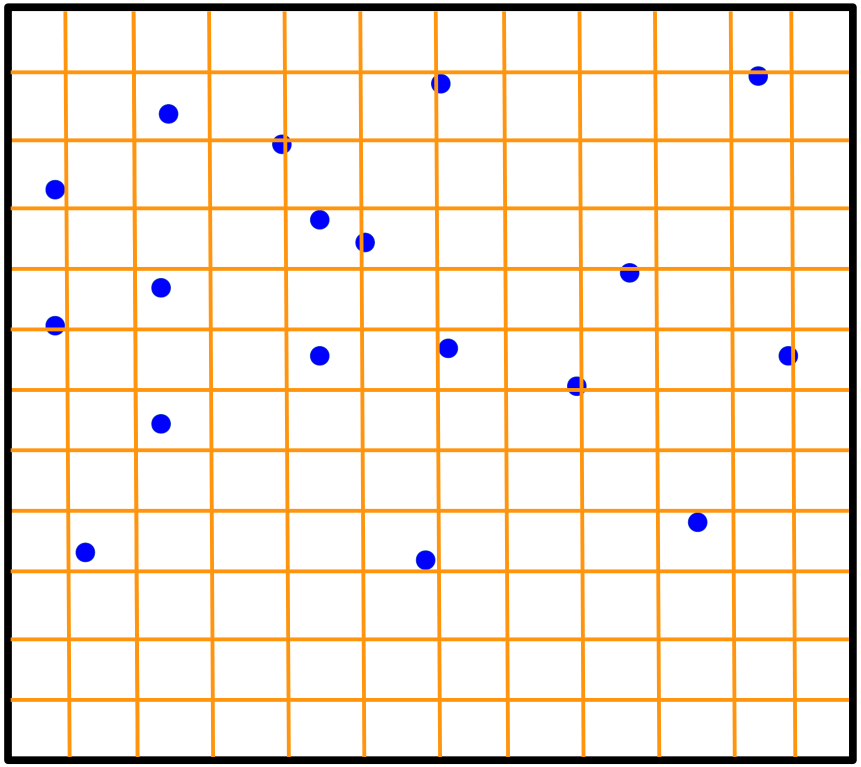

Lattice size: L

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Continuous limit: fix N, send L to infinite

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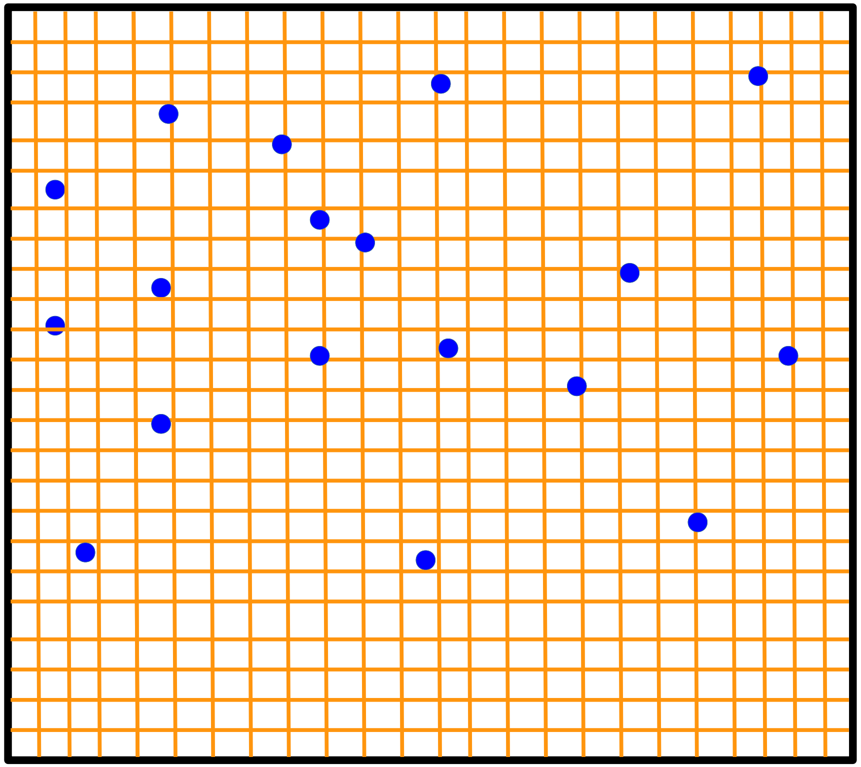

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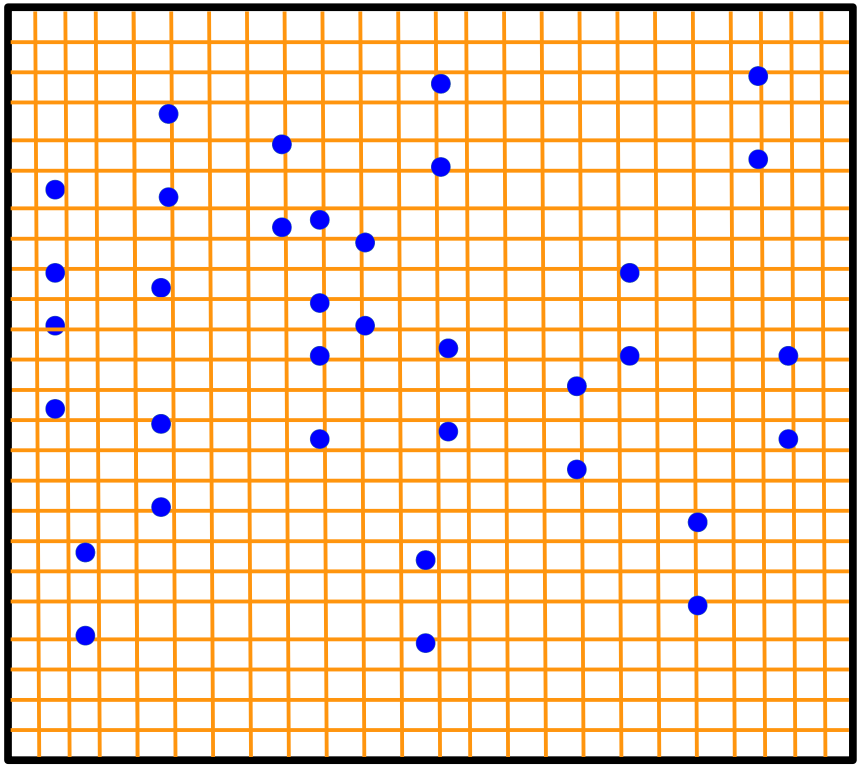

Particles in the box

Lattice size: L

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Continuous limit: fix N, send L to infinite

Thermodynamic limit: sent N to infinite

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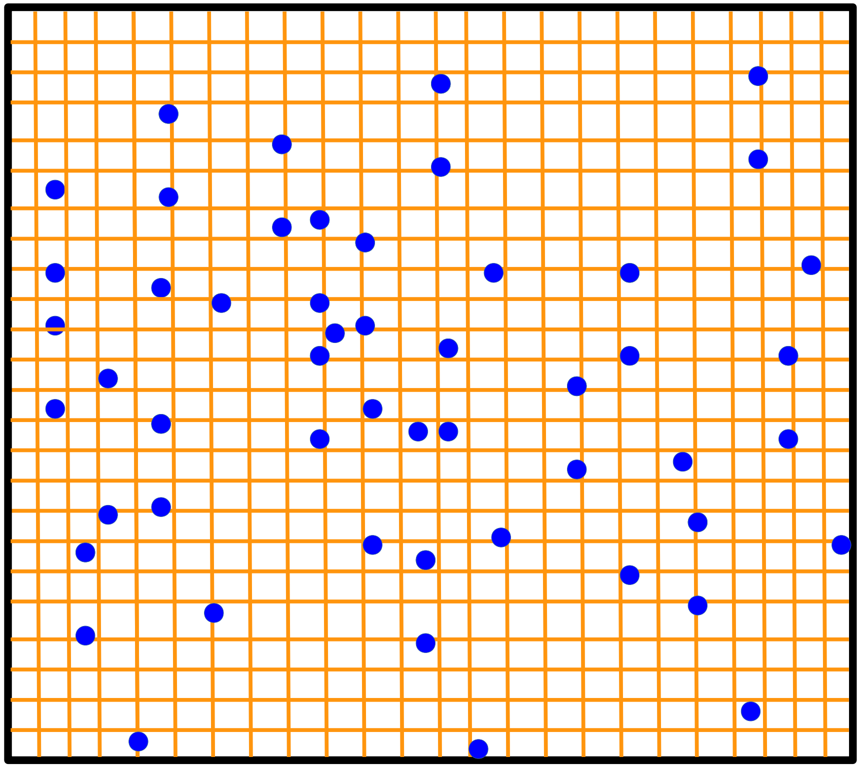


Lattice size: L

Number of particles: N

$$n = N/L$$

Particles in the box

For details on FG w/o SOC, see arXiv:1504.00925

Continuous limit: fix N, send L to infinite

Thermodynamic limit: sent N to infinite

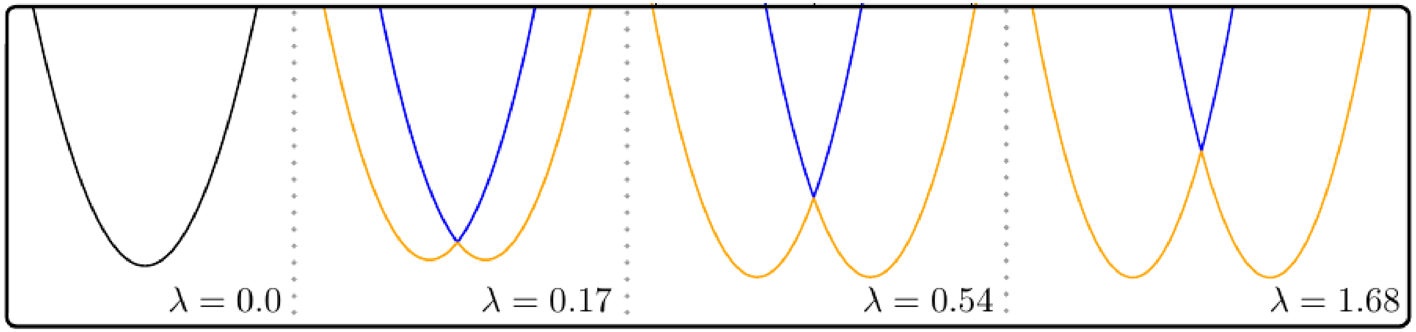
Non-Interacting Limit

$$H = \sum_{\mathbf{k}\sigma} k^2 c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + \sum_{\mathbf{k}} \lambda (k_y - i k_x) c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + h.c.$$

For U = 0 (i.e. non-interacting):

Diagonalization yields two bands →

$$\begin{cases} \varepsilon(\mathbf{k})_+ = k^2 + \lambda k \\ \varepsilon(\mathbf{k})_- = k^2 - \lambda k \end{cases}$$



increasing SOC strength →

Non-Interacting Limit

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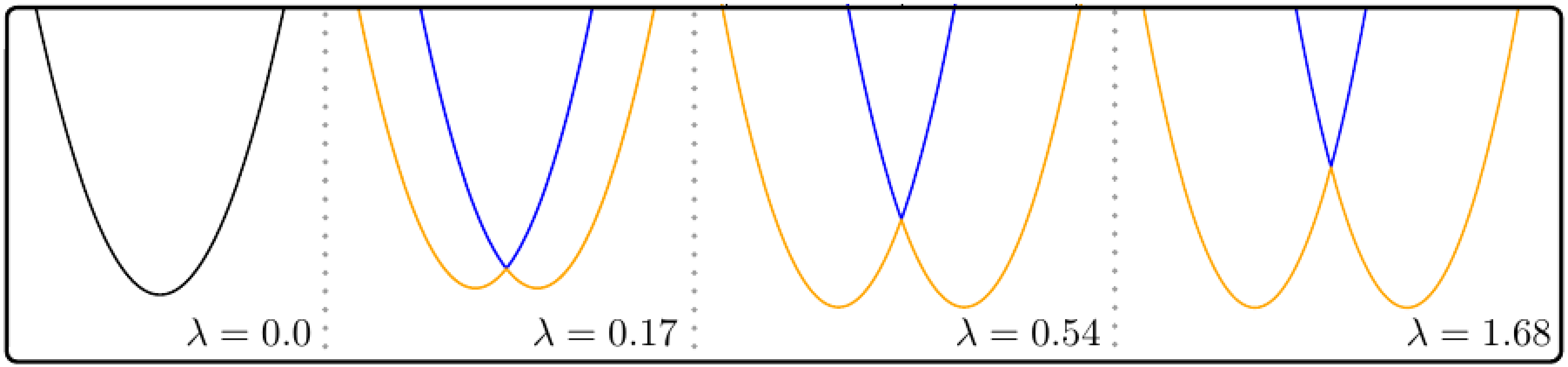

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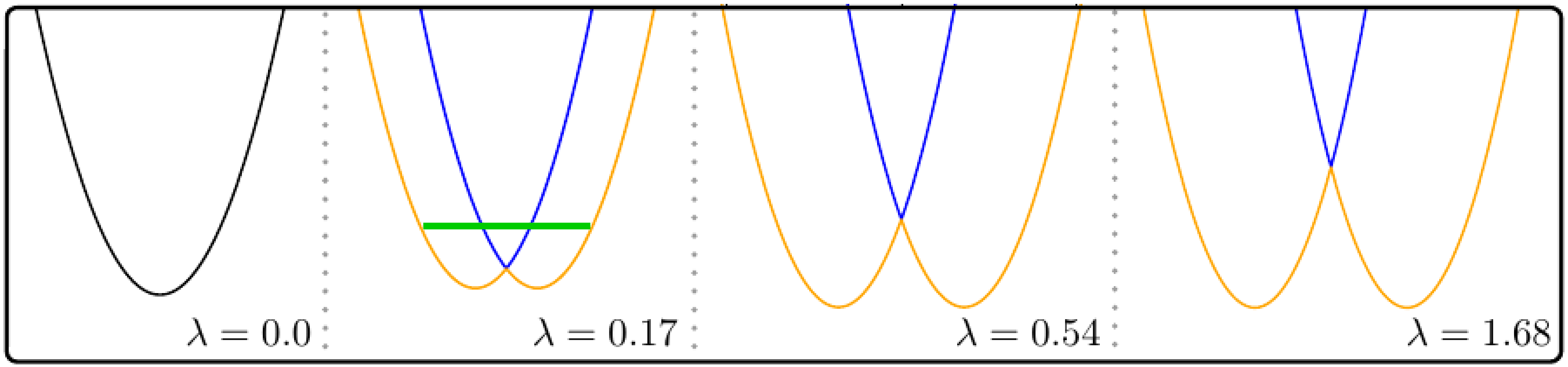

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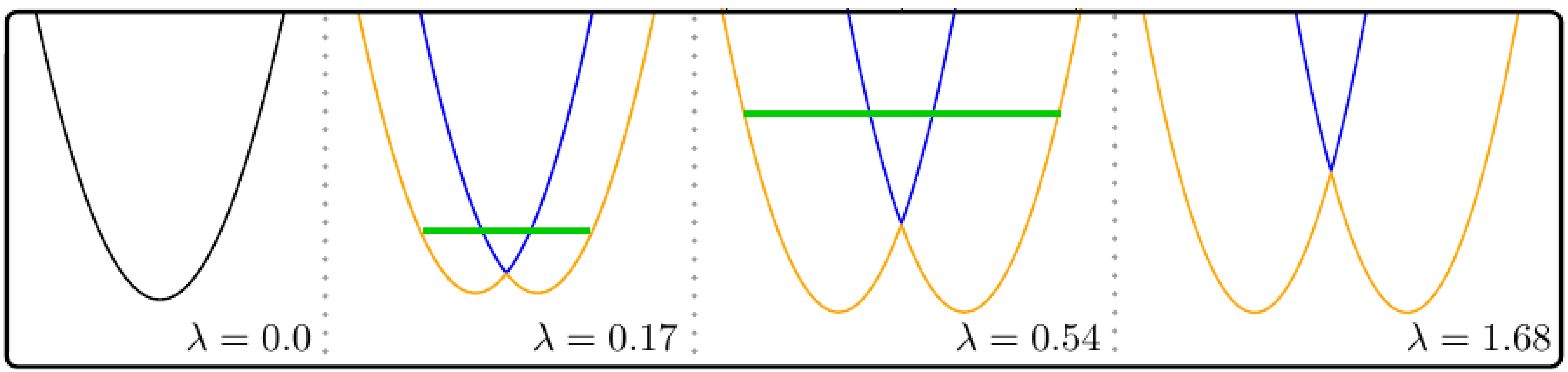

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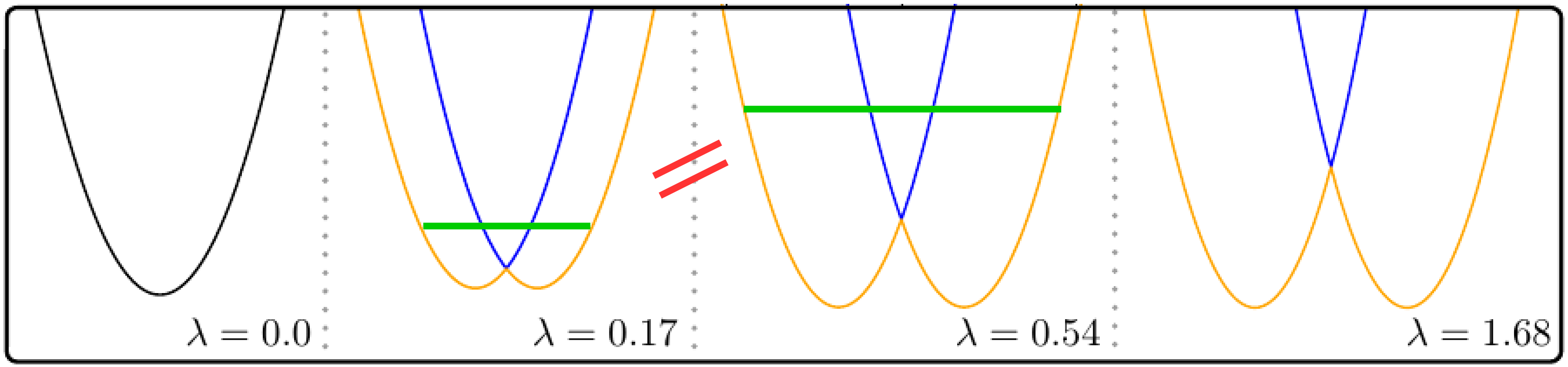


$\alpha = \lambda^2 / E_{FG}$ defines the spin-orbit coupling strength.

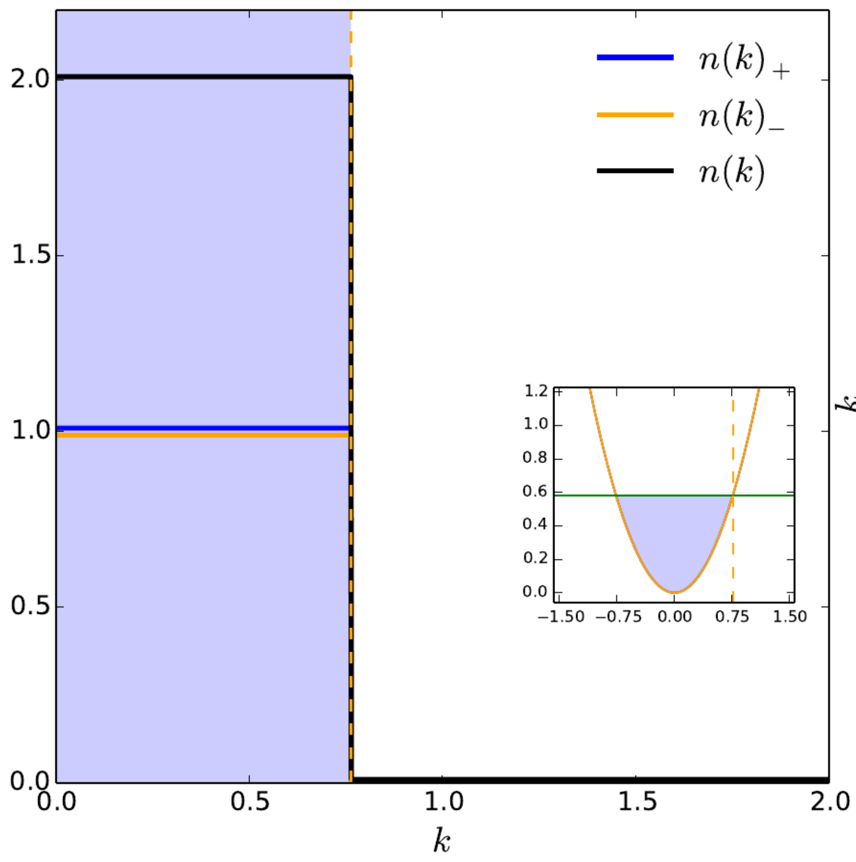
$$E_{FG} = \pi n$$

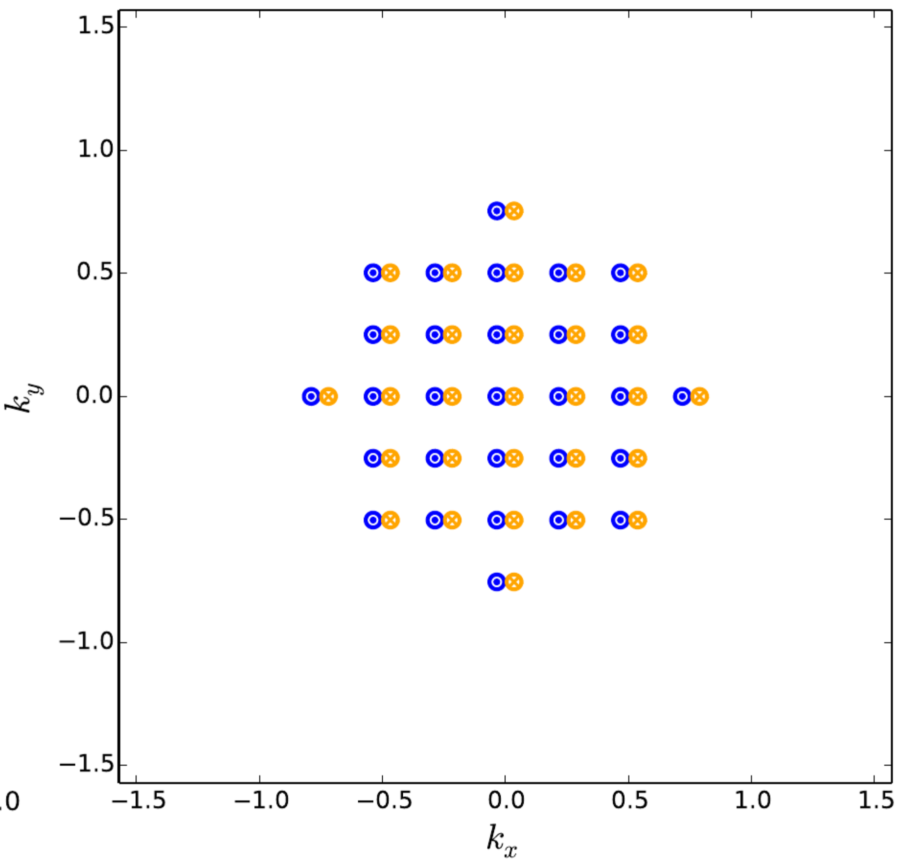
Momentum Distribution and Spin State

$$\alpha = 0.0$$

$$U = 0$$

$$\alpha = \lambda^2 / E_{FG}$$





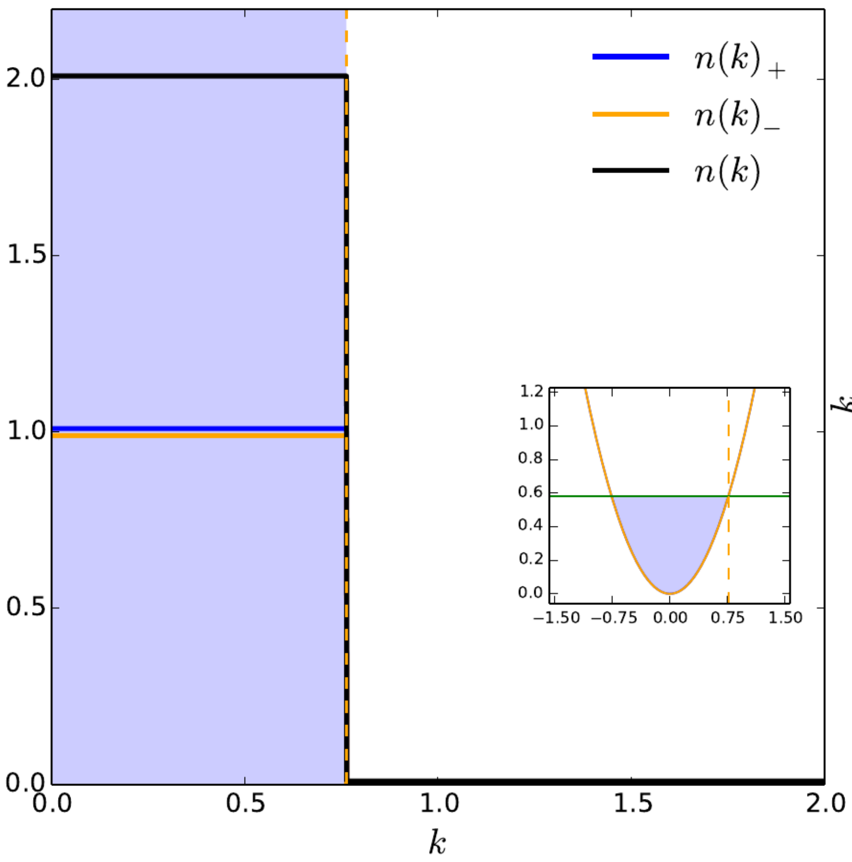
- With no SOC $\varepsilon(k)_+ = \varepsilon(k)_-$ the dispersion is the standard k^2.

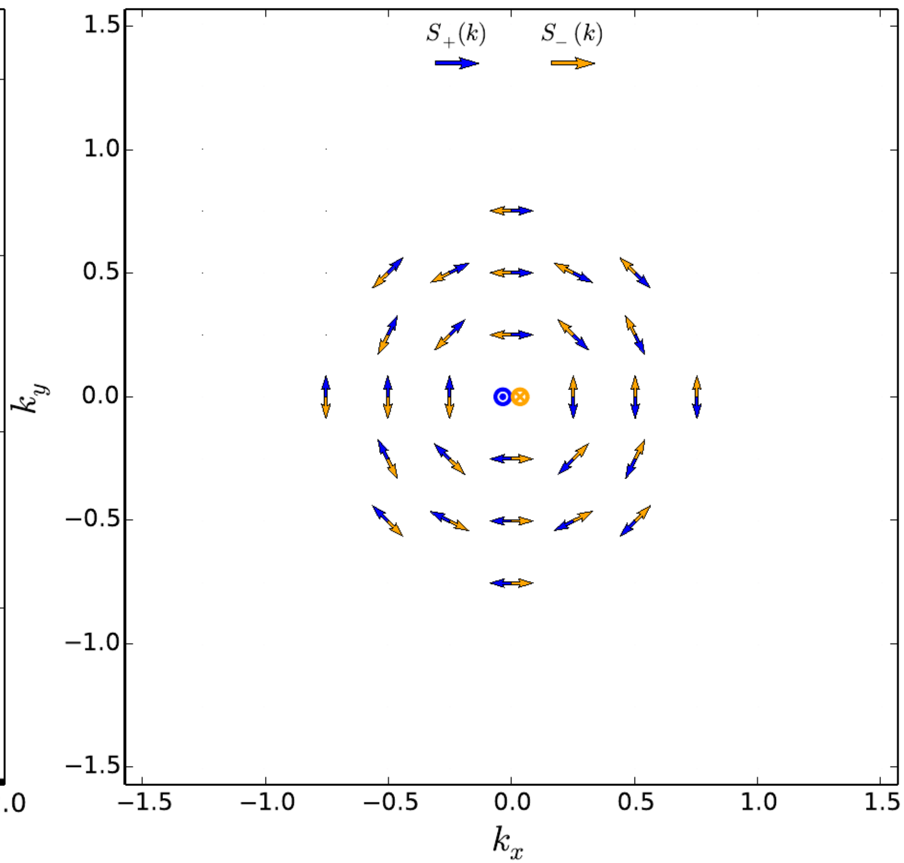
Momentum Distribution and Spin State

$$\alpha = 0.0^{+}$$

$$\boxed{U = 0}$$

$$\alpha = \lambda^2 / E_{FG}$$





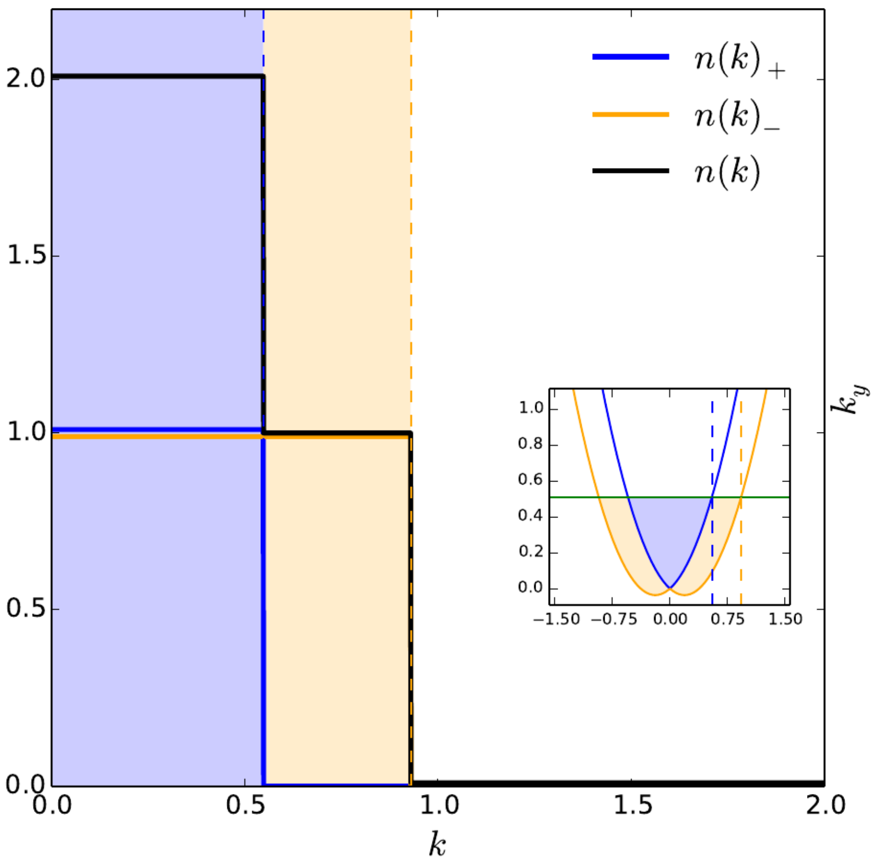
- As SOC strength increases, the dispersion separates into two distinct bands: $\varepsilon(k)_+$ and $\varepsilon(k)_-$
- Spin rotates in momentum space

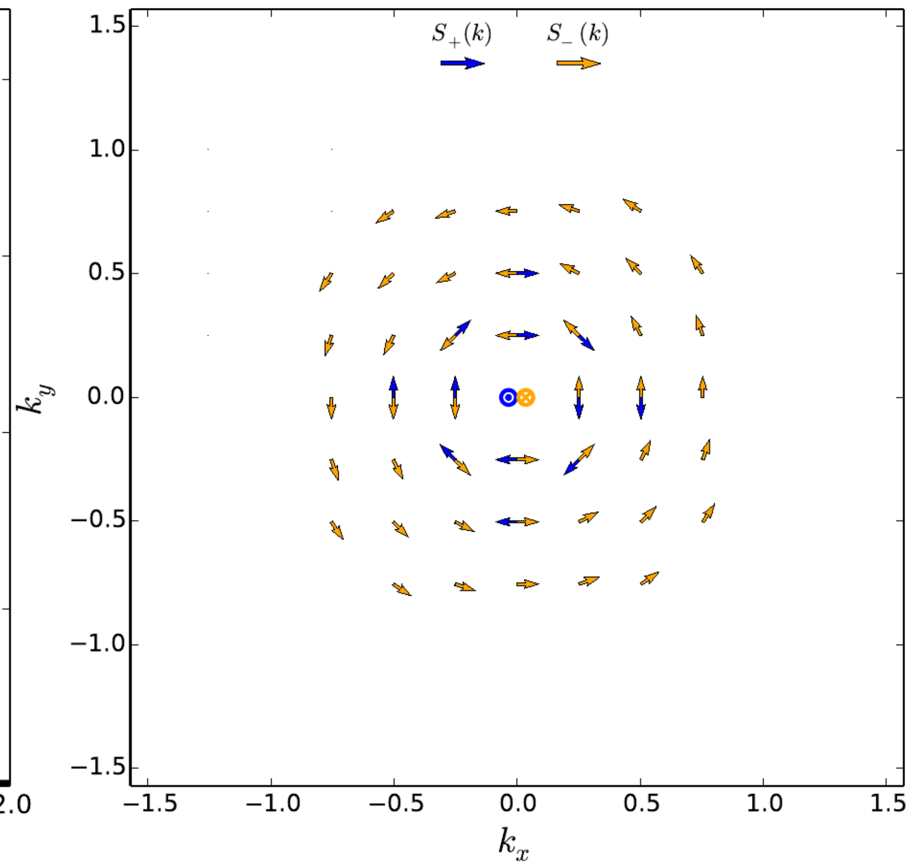
Momentum Distribution and Spin State

$$\alpha = 0.5$$

$$\boxed{U = 0}$$

$$\alpha = \lambda^2 / E_{FG}$$





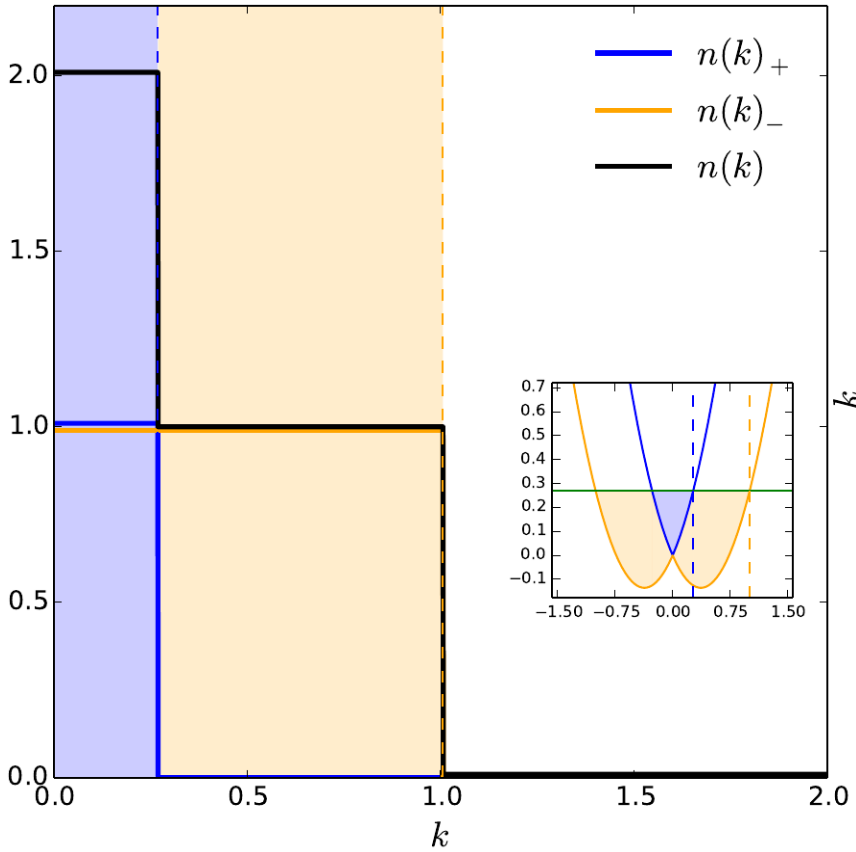
- As SOC strength increases, the region of k-space where $\varepsilon(k)_+$ is occupied shrinks.

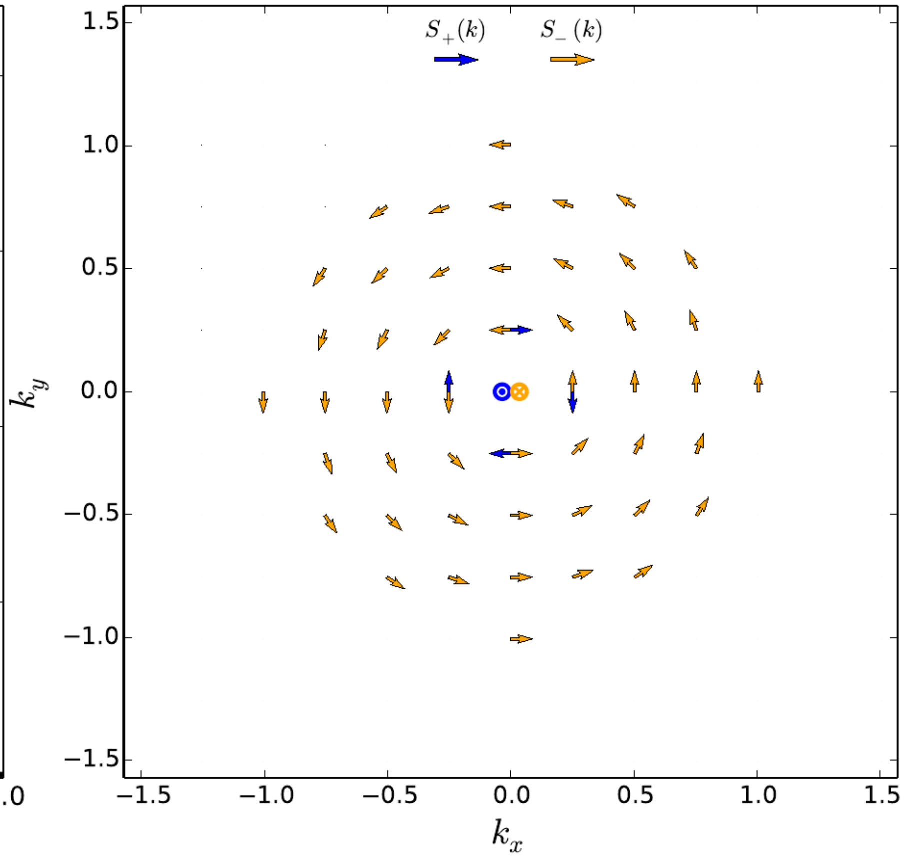
Momentum Distribution and Spin State

$$\alpha = 2.0$$

$$\boxed{U = 0}$$

$$\alpha = \lambda^2 / E_{FG}$$





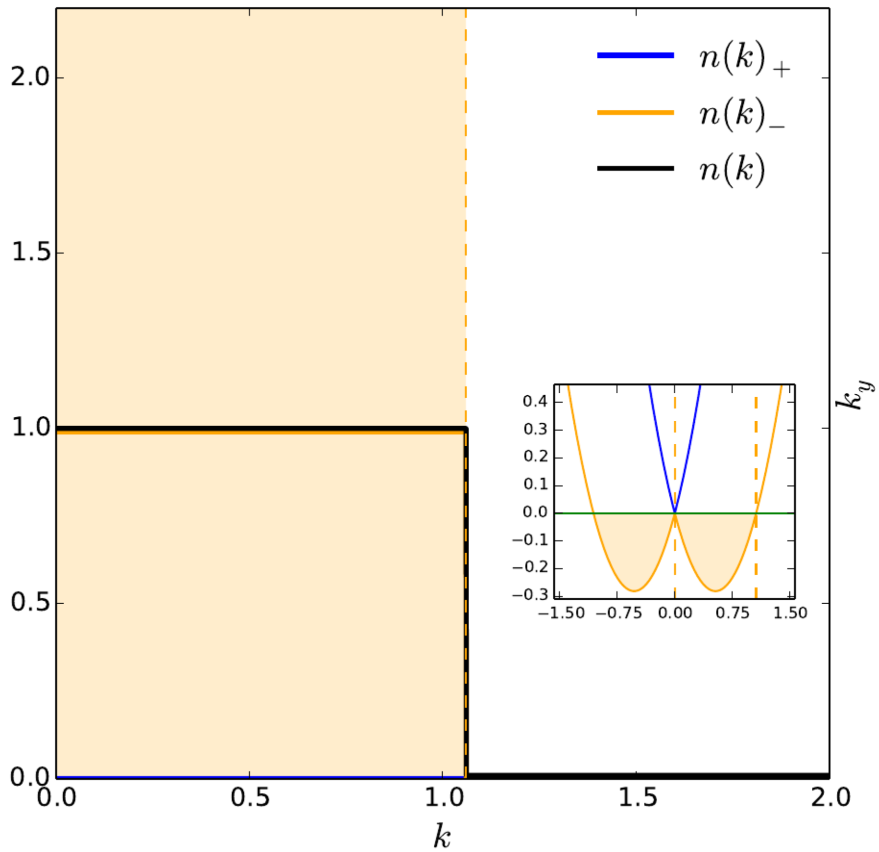
- As SOC strength increases, the region of k-space where $\varepsilon(k)_+$ is occupied shrinks.

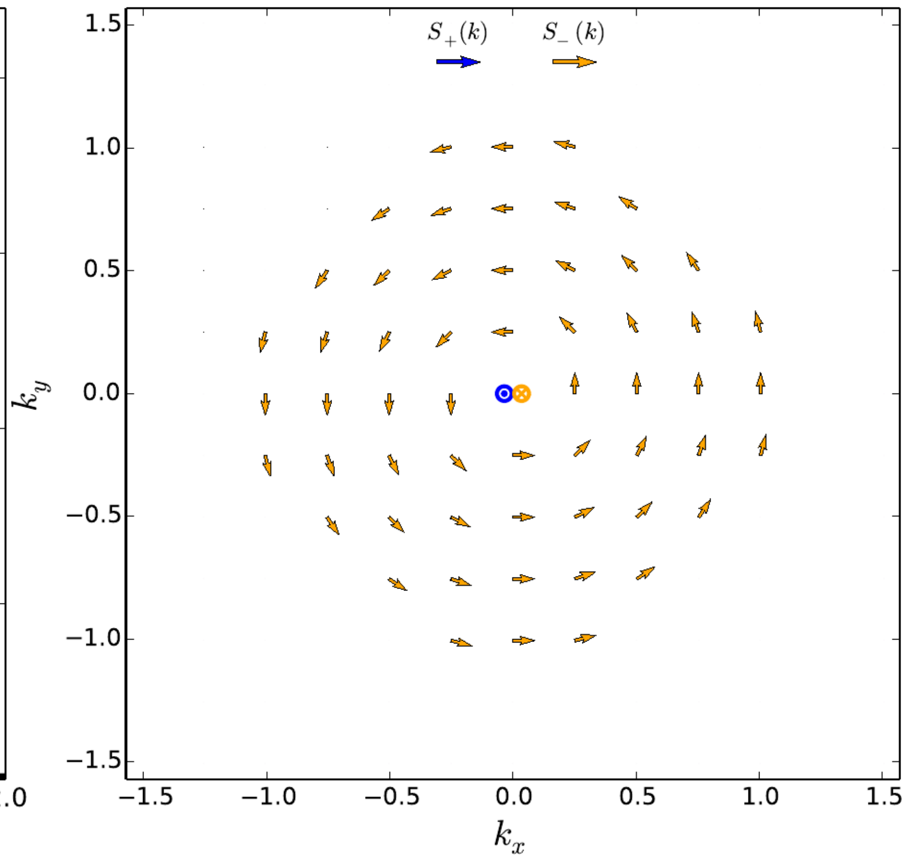
Momentum Distribution and Spin State

$$\alpha = 4.0$$

$$\boxed{U = 0}$$

$$\alpha = \lambda^2 / E_{FG}$$





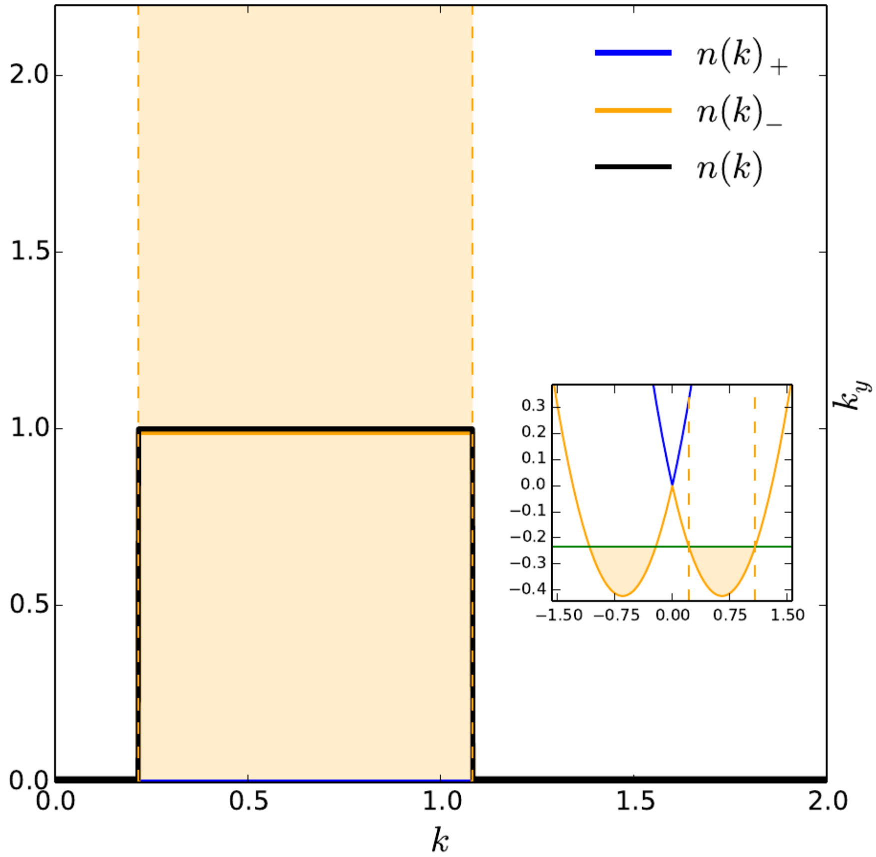
- Weak SOC to strong SOC transition

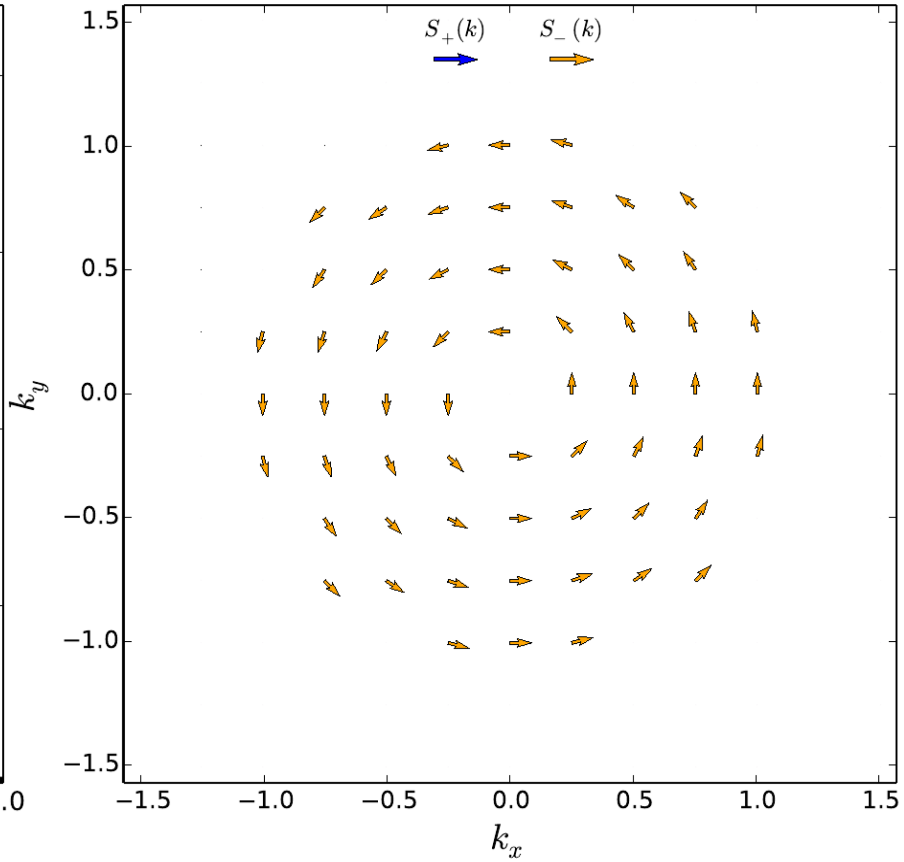
Momentum Distribution and Spin State

$$\alpha = 6.0$$

$$\boxed{U = 0}$$

$$\alpha = \lambda^2 / E_{FG}$$





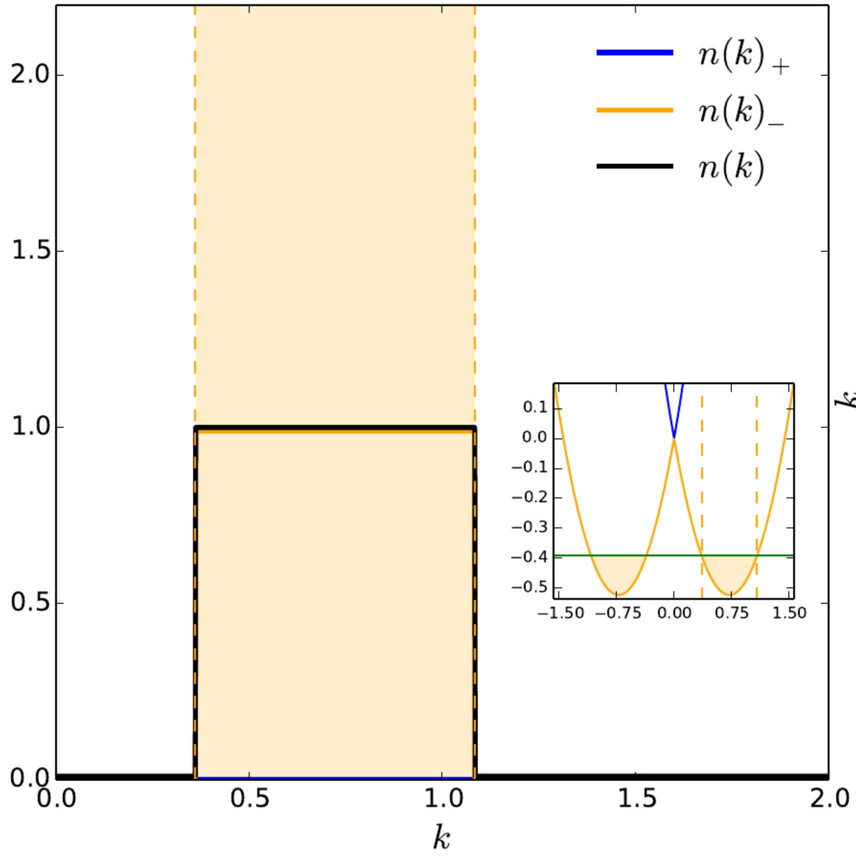
- Eventually for strong enough SOC, only the $\varepsilon(k)_-$ band is occupied.
- With increasing SOC strength, the region where $\varepsilon(k)_-$ is occupied moves away from k=0, and shrinks.

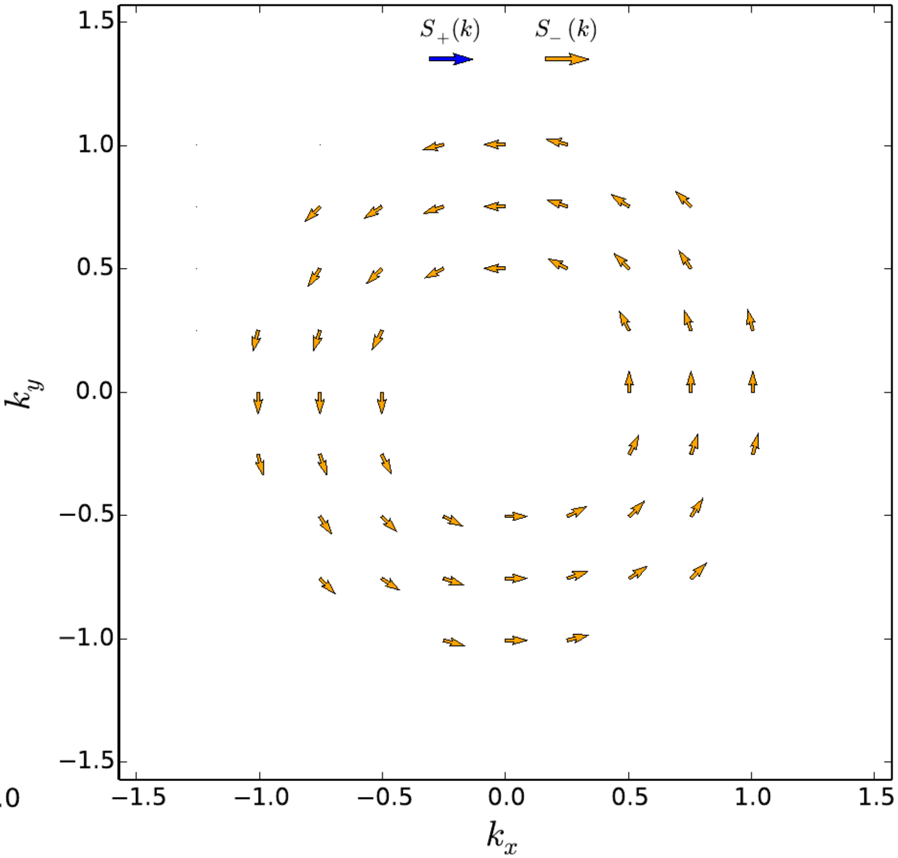
Momentum Distribution and Spin State

$$\alpha = 8.0$$

$$U = 0$$

$$\alpha = \lambda^2 / E_{FG}$$





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Momentum Distribution and Spin State

$$\alpha = 8.0$$

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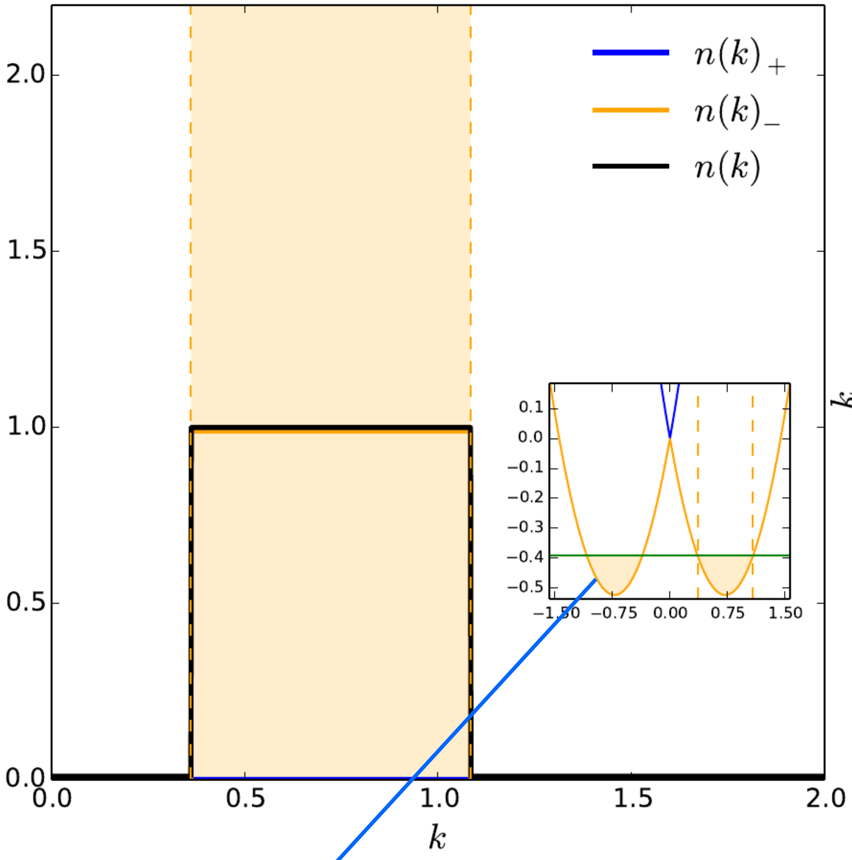
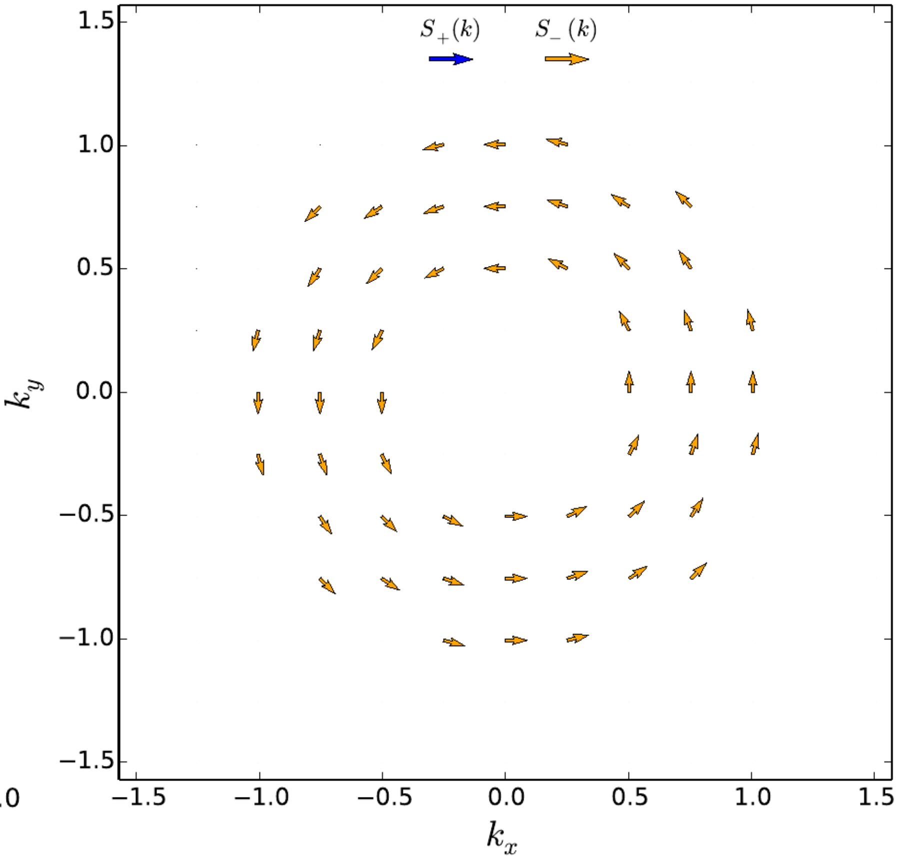
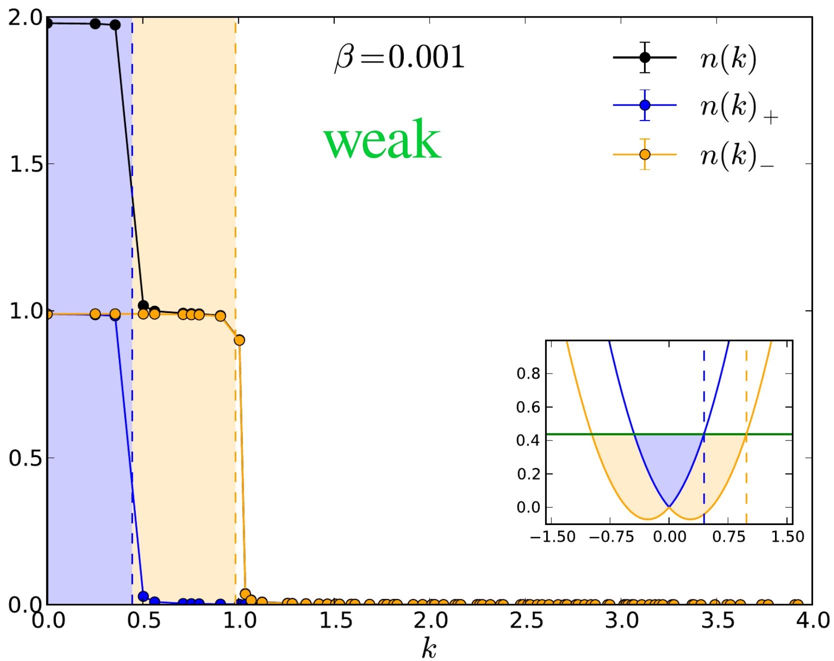


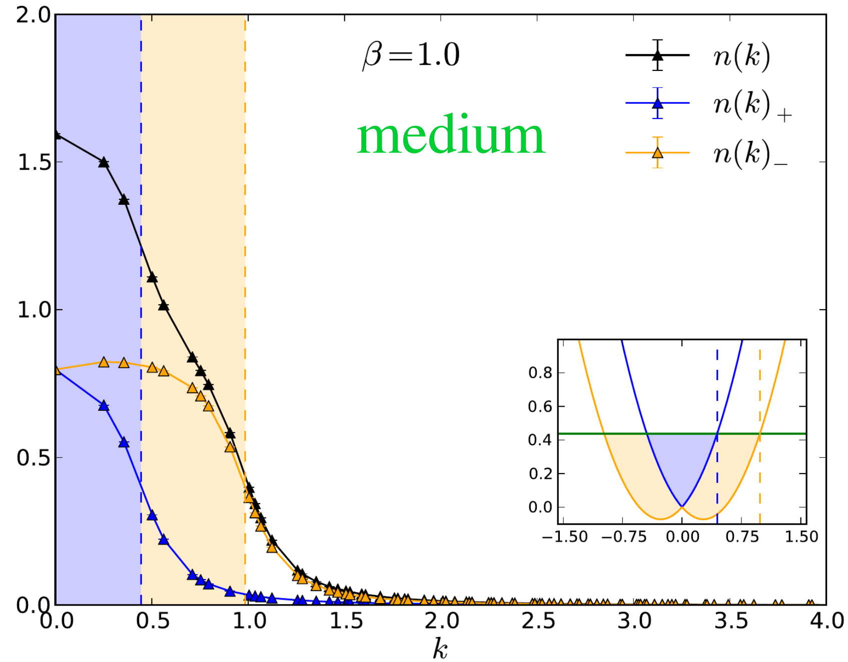


- With increasing SOC strength, the region where $\varepsilon(k)_-$ is occupied moves away from k=0, and shrinks.

Effective 1D density of states, enhances quantum fluctuations!

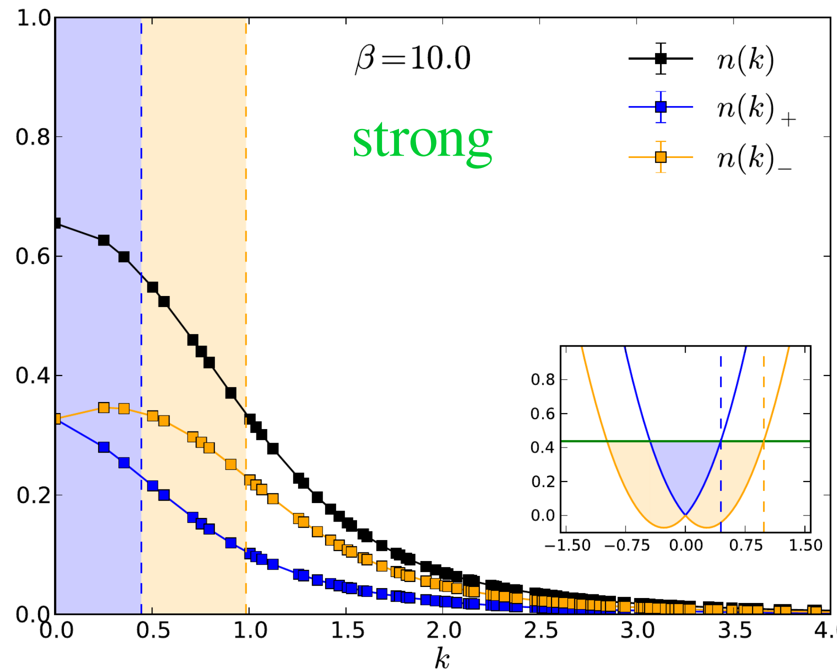
Momentum Distribution with Interaction





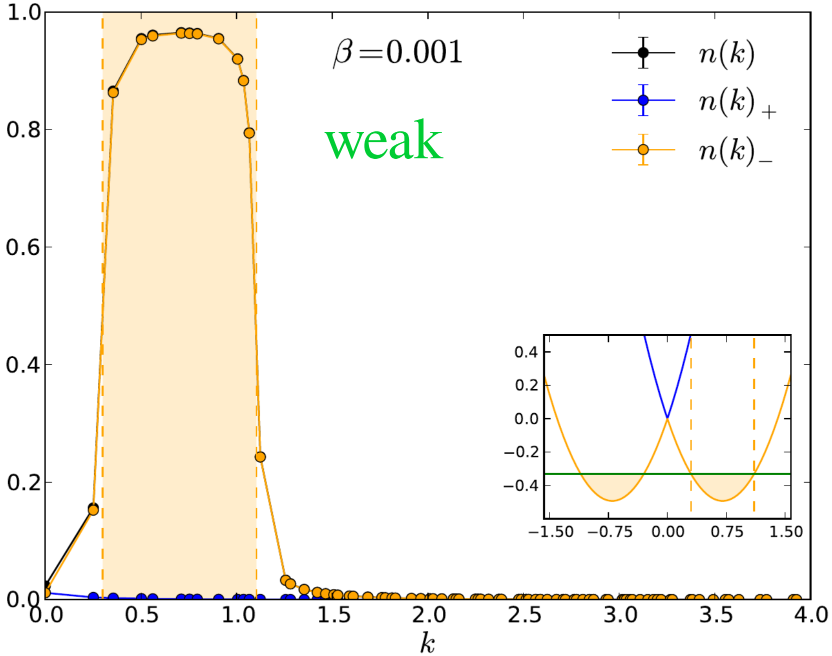
- In weak SOC regime, both bands are occupied.
- As interaction strength increases, occupation spreads to higher k

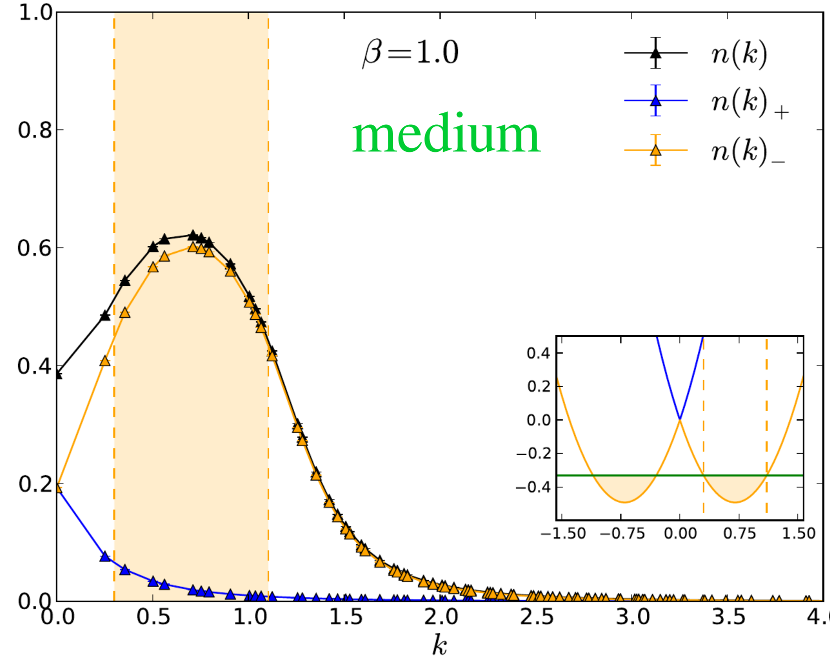
L=625, N=56 $\alpha = 1.0$



preliminary

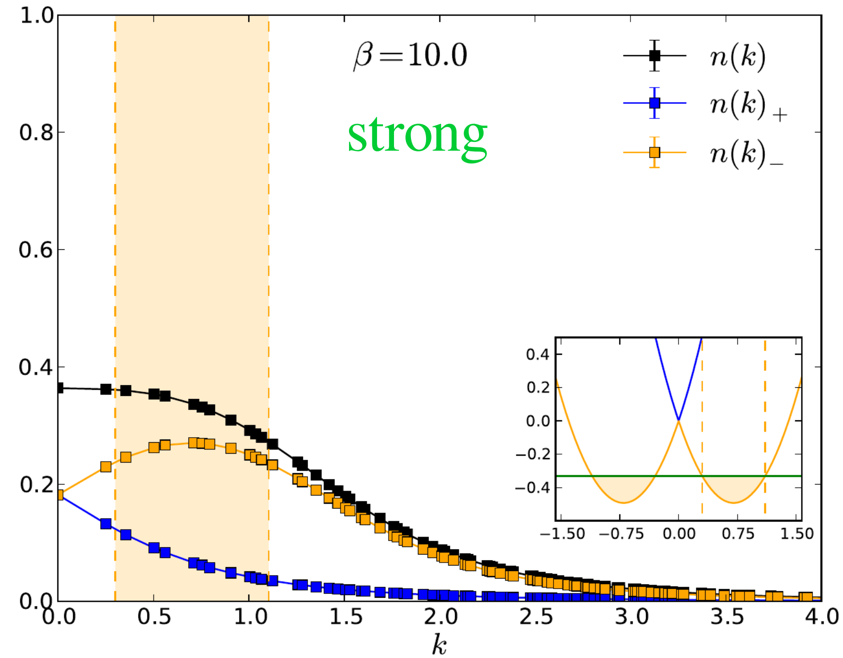
Momentum Distribution with Interaction





- In strong SOC regime, only the lower band is occupied.
- As interaction strength increases, occupation spreads to higher k and higher band.

L=625, N=56 $\alpha = 7.0$



Singlet and Triplet Paring

- Singlet pairing

$$\Delta_s^\dagger(k) = \frac{1}{2}(c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{-k\uparrow}^\dagger)$$

- Triplet pairing

$$\Delta_\uparrow^\dagger(k) = c_{k\uparrow}^\dagger c_{-k\uparrow}^\dagger \quad \Delta_\downarrow^\dagger(k) = c_{k\downarrow}^\dagger c_{-k\downarrow}^\dagger$$

- Pairing matrix

$$M(k\sigma, k'\sigma') = \Delta_\sigma^\dagger(k)\Delta_{\sigma'}(k')$$

3Lx3L matrix

Outline

- Introduction to AFQMC
  - Release constraint
  - Symmetry in trial wave function
  - Generalized Hartree–Fock (GHF) wave function
- Magnetic orders in 2D Hubbard model — GHF trial wave function
  - Half-filling: restores symmetry
  - Doped: more accurate results
- Rashba spin-orbit coupling in 2D Fermi gas — GHF random walker
  - Interplay between SOC and interaction
  - Singlet triplet pairing wave function
- **Conclusion**

Conclusion

- Systematically improvable AFQMC method

  - Release constraint
  - Symmetry in trial wave function
  - Generalized Hartree–Fock (GHF) trial wave function

- Magnetic orders in 2D Hubbard model

  - GHF trial wave function restores symmetry at half-filling
  - GHF trial wave function gives more accurate result in the doped (magnetic), strongly correlated region.

- Rashba spin-orbit coupling in 2D Fermi gas Ongoing!

  - GHF random walkers
  - Interplay between SOC and strong interaction
  - Singlet and triplet pairing

For details on FG w/o SOC, see arXiv:1504.00925