Spin Symmetry and the
Graphical Unitary Group Approach

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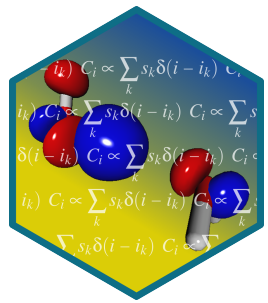
Stuttgart, June 20, 2017



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Symmetries

Noether-Theorem: Symmetry $\leftrightarrow$ Conservation law

$$[\hat{H}, \hat{O}] = 0$$

- Gauge invariance, Time reversal-, Translational and Rotational Symmetry

Symmetries routinely used in Electronic structure calculations:

- Translational symmetry: momentum space basis
- S_z symmetry: fix m_s value of SD
- Point Group Symmetry: Stay in same irrep of P_G

Symmetry adapted basis: invariant and irreducible under $\hat{O}$

SU(2) spin symmetry

Total spin symmetry: inherent to spin-preserving, non-relativistic Hamiltonians:

$$[\hat{H}, \hat{S}^2] = 0$$

usually neglected, due to *impractical implementation.*
Symmetry adapted basis:

- target specific spin-states (singlet, triplet)
- no spin-contamination
- reduce Hilbert space size!
- lift degeneracies of different spin-sectors

$\rightarrow$ **Configuration state functions (CSFs)**

Roadmap to CSFs in the UGA

- n spatial and $2n$ spin-orbitals in $\hat{H}$
- Goal in the UGA: total anti-symmetric representation of $U(2n)$
- Ensured by direct product $U(2n) = U(n) \otimes U(2)$ of spatial part U(n) and spin U(2) part
- Express $\hat{H}$ in terms on generators of $U(n)$ and specify irreps and symmetry adapted basis thereof (CSFs)
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Eg. Two-particles:
-antisymmetric spin function $(\alpha\beta - \beta\alpha)$ forces symmetric spatial function $\rightarrow$ *singlet* state
-symmetric spin functions $(\alpha\alpha, \alpha\beta + \beta\alpha, \beta\beta)$ force anti-symmetric spatial function $\rightarrow$ *triplet* states

Spin-free formulation

of a spin-preserving, non-relativistic Hamiltonian:

$$\hat{H} = \sum_{ij}^{n} \sum_{\sigma=\uparrow,\downarrow} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{ijkl}^{n} \sum_{\sigma,\tau=\uparrow,\downarrow} [ij;kl] c^{\dagger}_{i\sigma} c^{\dagger}_{k\tau} c_{l\tau} c_{j\sigma}$$

Spin-preserving substitution operators: $\boxed{E_{ij} = c^{\dagger}_{i\uparrow} c_{j\uparrow} + c^{\dagger}_{i\downarrow} c_{j\downarrow}}$ With

$$c^{\dagger}_{i\sigma} c^{\dagger}_{k\tau} c_{l\tau} c_{j\sigma} = c^{\dagger}_{i\sigma} c_{j\sigma} c^{\dagger}_{k\tau} c_{k\tau} - \delta_{jk} \delta_{\sigma\tau} c^{\dagger}_{i\sigma} c_{l\sigma}$$

We have

$$\sum_{\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} = E_{ij}, \quad \sum_{\sigma\tau} c^{\dagger}_{i\sigma} c^{\dagger}_{k\tau} c_{l\tau} c_{j\sigma} = E_{ij} E_{kl} - \delta_{jk} E_{il}$$

We get:

$$\boxed{\hat{H} = \sum_{ij}^{n} t_{ij} E_{ij} + \frac{1}{2} \sum_{ijkl}^{n} [ij;kl] \left(E_{ij} E_{kl} - \delta_{jk} E_{il} \right)}$$

Commutation relations:

Commutator:

$$
\begin{aligned}
[E_{ij}, E_{kl}] &= \sum_{\sigma\tau} c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\tau} c_{l\tau} - c^\dagger_{k\tau} c_{l\tau} c^\dagger_{i\sigma} c_{j\sigma} \\
&= \sum_{\sigma\tau} \cdots - c^\dagger_{i\sigma} c^\dagger_{k\tau} c_{l\tau} c_{j\sigma} - \delta_{il} c^\dagger_{k\tau} c_{j\sigma} \\
&= \sum_{\sigma\tau} \cancel{c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\tau} c_{l\tau}} - \cancel{c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\tau} c_{l\tau}} + \delta_{jk} c^\dagger_{i\sigma} c_{l\tau} - \delta_{il} c^\dagger_{k\tau} c_{j\sigma}
\end{aligned}
$$

$$
\boxed{[E_{ij}, E_{kl}] = \delta_{jk} E_{il} - \delta_{il} E_{kj}}
$$

The Unitary Group U(n)

- group of all $n \times n$ unitary matrices: $U^\dagger U = 1$
- Simple case U(1): all complex numbers z with $|z| = 1$
- Continous, real Lie group of dimension n^2
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basic matrix units $\mathbf{e_{ij}}$: only one non-vanishing element (1) at (i, j)

$$\boxed{[\mathbf{e_{ij}}, \mathbf{e_{kl}}]} = \mathbf{e_{ij}}\mathbf{e_{kl}} - \mathbf{e_{kl}}\mathbf{e_{ij}} \boxed{= \delta_{jk}\mathbf{e_{il}} - \delta_{il}\mathbf{e_{kj}}}$$

This is the important relation between the **unitary group** and **electronic structure theory!**

Irreps of U(n)

Two key ideas in the UGA:

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First step: Identify and uniquely specify the **irreps** of U(n)!

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First step: Identify and uniquely specify the **irreps** of U(n)!
Analogy: group of rotations in 3D SO(3) and spherical Harmonics:

$$[\hat{L}^2, \hat{L}_z] = 0, \quad \hat{L}^2 Y_{lm} = l(l+1) Y_{lm}, \quad \hat{L}_z Y_{lm} = m_l Y_{lm}$$

Casimir operator of SO(3) $\hat{L}^2$: $[\hat{L}^2, \hat{L}_i] = 0$, $i = x, y, z$
$\hat{L}_z$ Casimir operator and generator of rotations in 2D: SO(2)

Group subduction chain

Y_{lm} symmetry adapted to group chain:

$$SO(3) \supset SO(2)$$

- **Irrep of SO(3)** specified by $\hat{L}^2$ eigenvalue l
- **Basis states** Y_{lm} of irrep labeled by $\hat{L}_z$ eigenvalue m_l

$$-l \leq m_l \leq l$$

Y_{lm}: invariant and irreducible under action of generators of SO(3):

$$\hat{L}_i \, Y_{lm} = \sum_{m'=-l}^{l} c_{m'} \, Y_{lm'}$$

Irreps of U(n)

Similar to Y_{lm} the GT basis is based on the chain of subgroups:

$$U(n) \supset U(n-1) \supset \cdots \supset U(2) \supset U(1)$$

But U(n) has n^2 generators E_{ij} and n Casimir operators

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- **Irrep of U(n)** specfied by n eigenvalues:
  $\mathbf{m_n} = (m_{1n}, \ldots, m_{nn}), \quad m_{1,n} \geq m_{2,n} \geq \cdots \geq m_{n,n}$

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Arrange the eigenvalues of the Casimir operators:

$$\begin{array}{ccccccccccc}
U(n) & & m_{1n} & & & m_{2n} & \cdots & m_{n-1,n} & & & m_n \\
U(n-1) & & & m_{1,n-1} & & & \cdots & & m_{n-1,n-1} & & \\
\ldots & : & & & & & \cdots & & & & \\
U(2) & & & & & m_{12} & & m_{22} & & & \\
U(1) & & & & & & m_{11} & & & &
\end{array}$$

Example: U(2) - Spin part

$$\begin{array}{lccc} U(2): & m_{12} & & m_{22} \\ U(1): & & m_{11} & \end{array} \qquad m_{12} \geq m_{11} \geq m_{22}$$

Irreps labeled by top row: $m^S = (m_{12}, m_{22})$

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Single particle of spin-1/2: $m^S = (1, 0)$:

$$|\uparrow\rangle = \begin{array}{cc} 1 & 0 \\ & 1 \end{array} \qquad |\downarrow\rangle = \begin{array}{cc} 1 & 0 \\ & 0 \end{array}$$

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$S=1$						$S=0$	
$m_s=1$		$m_s=0$		$m_s=-1$		$m_s=0$	
2	0	2	0	2	0	1	1
2		1		0		1	
$\|\uparrow\uparrow\rangle$		$\|\uparrow\downarrow\rangle + \|\downarrow\uparrow\rangle$		$\|\downarrow\downarrow\rangle$		$\|\uparrow\downarrow\rangle - \|\downarrow\uparrow\rangle$	

Young shapes and Weyl Tableaux

We can identify:

- Total particle number: $N = m_{12} + m_{22}$
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Pictorial representation:

- Irrep: **Young shape** - N boxes, m_{12} in first row, m_{22} in second
- Basis states: **Weyl Tableau** - filled with "tokens" (spins)

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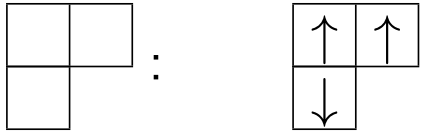
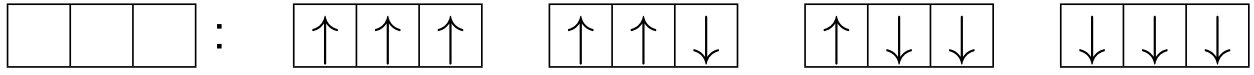
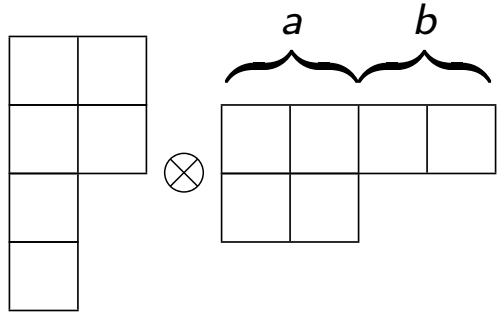
N = 3 particles: $m_1^S = (2,1), \quad m_2^S = (3,0)$

$S = 1/2$: 

$S = 3/2$: 

$U(2n) = U(n) \otimes U(2)$

- Spin-free formulation of H $\rightarrow$ U(2) only determines Young shape of spatial U(n)
- Irreps of U(n): $m_{ij} \leq 2 \rightarrow$ max. two colums
- Total anti-symmetric representation of $U(2n) = U(n) \otimes U(2)$:



- Total spin $S = b/2$, Number of electrons $N = 2a + b$, Number of spatial orbitals n

2 electrons in 3 spatial orbitals

U(3) irreps determined by spin-state: Fill in orbital "tokens":
(1,2,3) with no repetitions in same column to get **CSFs**:

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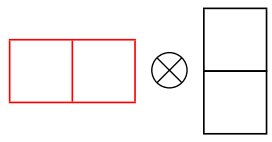
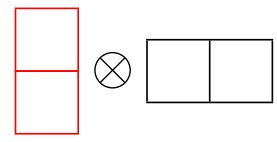
$S = 0$: 

$S = 1$: 

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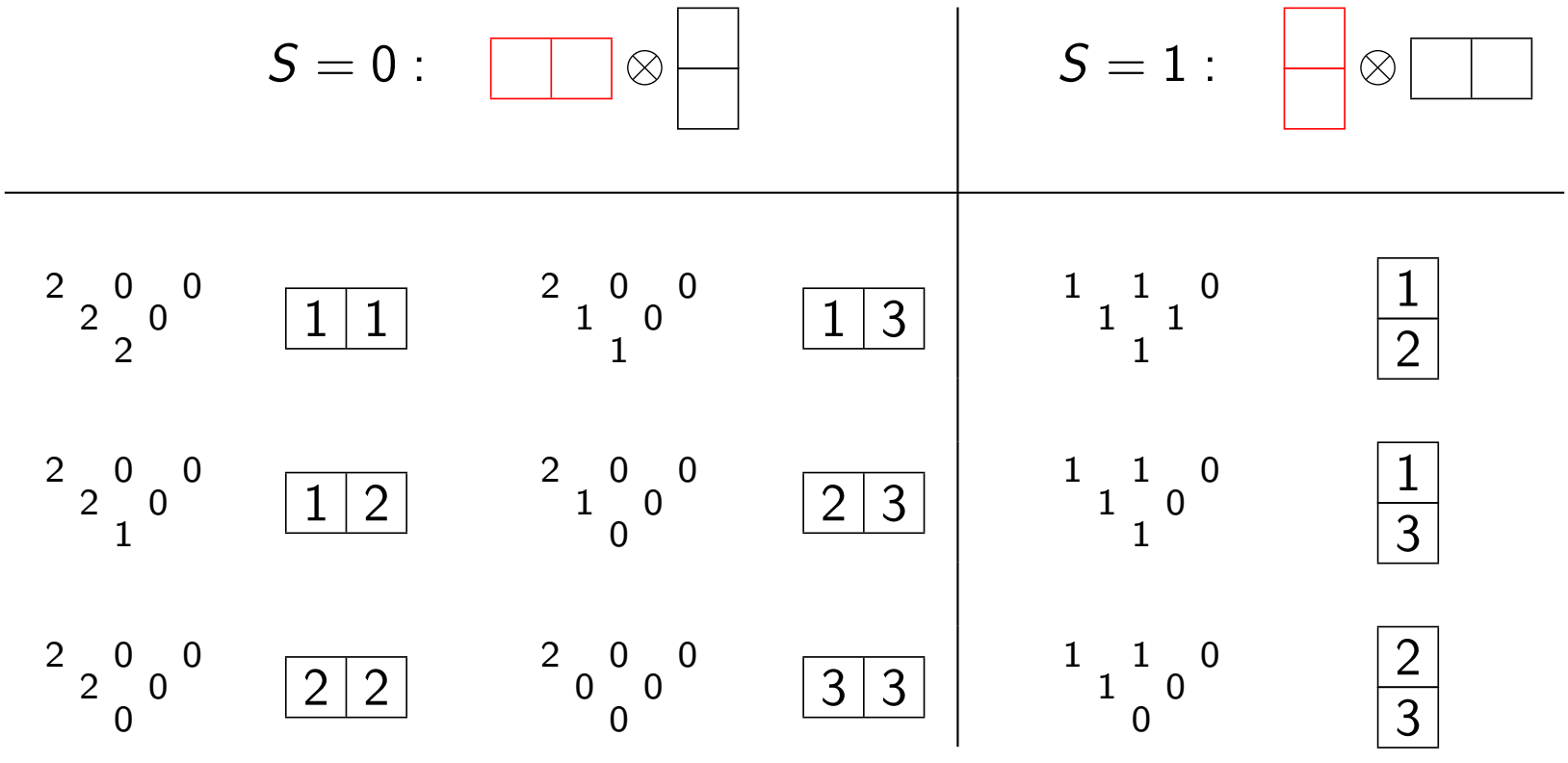
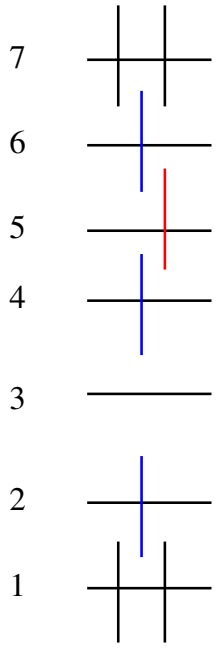


Sequential orbital coupling in UGA

Example:
$N = 8$ electrons in $n = 7$ spatial orbitals with total spin $S = 1$
One possible **CSF:**



1	1
2	5
4	7
6	
7	

Sequential orbital coupling in UGA

1	1
2	5
4	7
6	
7	

Start with Null entry at bottom of the table

orbital (i)	a_i	b_i	N_i	S_i	d_i
7	3	2	8	1	3
6	2	2	6	1	1
5	2	1	5	$1/2$	2
4	1	2	4	1	1
3	1	1	3	$1/2$	0
2	1	1	3	$1/2$	1
1	1	0	2	0	3
0	0	0	0	0	

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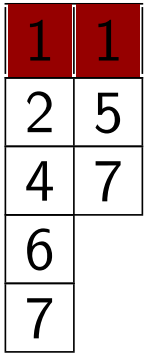

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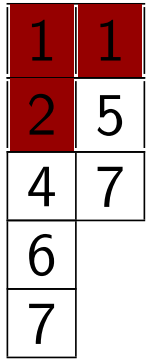
6	2	2	6	1	1
5	2	1	5	1/2	2
4	1	2	4	1	1
3	1	1	3	1/2	0
2	1	1	3	1/2	1
1	1	0	2	0	3
0	0	0	0	0	

Adding orbital 1:
d_i is the *step number*
$d_1 = 3$: doubly occupied orbital

Sequential orbital coupling in UGA



Adding orbital 2:
$d_2 = 1$: singly ocucpied orbital, raising S_i by $1/2$

orbital (i)	a_i	b_i	N_i	S_i	d_i
7	3	2	8	1	3
6	2	2	6	1	1
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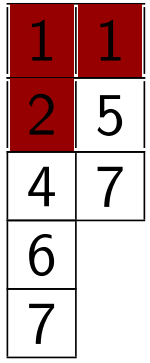

Adding orbital 3:
$d_3 = 0$: empty orbital,
no change in S_i

orbital (i)	a_i	b_i	N_i	S_i	d_i
7	3	2	8	1	3
6	2	2	6	1	1
5	2	1	5	1/2	2
4	1	2	4	1	1
3	1	1	3	1/2	0
2	1	1	3	1/2	1
1	1	0	2	0	3
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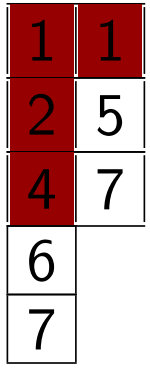
Sequential orbital coupling in UGA



Adding orbitals 4:
$d_4 = 1$ singly ocucpied orbital, raising S_i by $1/2$

orbital (i)	a_i	b_i	N_i	S_i	d_i
7	3	2	8	1	3
6	2	2	6	1	1
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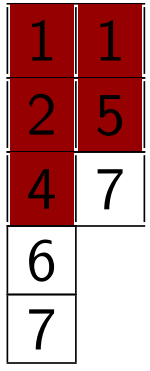
Sequential orbital coupling in UGA



Adding orbital 5:
$d_5 = 2$: singly occupied orbital, lowering S_i by $1/2$

orbital (i)	a_i	b_i	N_i	S_i	d_i
7	3	2	8	1	3
6	2	2	6	1	1
5	2	1	5	$1/2$	2
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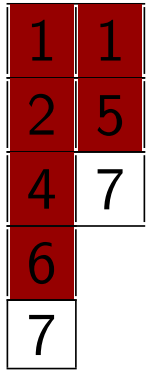

Adding orbitals 6:
$d_6 = 1$ singly ocucpied orbital, raising S_i by $1/2$

orbital (i)	a_i	b_i	N_i	S_i	d_i
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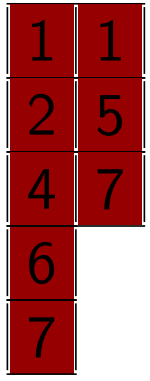
4	1	2	4	1	1
3	1	1	3	$1/2$	0
2	1	1	3	$1/2$	1
1	1	0	2	0	3
0	0	0	0	0	

Sequential orbital coupling in UGA



Adding orbitals 8:
$d_7 = 1$ doubly occupied orbital, no change in S_i

orbital (i)	a_i	b_i	N_i	S_i	d_i
7	3	2	8	1	3
6	2	2	6	1	1
5	2	1	5	1/2	2
4	1	2	4	1	1
3	1	1	3	1/2	0
2	1	1	3	1/2	1
1	1	0	2	0	3
0	0	0	0	0	

Step vector representation

Step-vector: most efficient CSF encoding

$$|\mathbf{d}\rangle = |3, 1, 0, 1, 2, 1, 3\rangle$$

2 bits per spatial orbital $\rightarrow$ same as Slater Determinants!

orbital (i)	a_i	b_i	N_i	S_i	d_i
7	3	2	8	1	3
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5	2	1	5	$1/2$	2
4	1	2	4	1	1
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2	1	1	3	$1/2$	1
1	1	0	2	0	3
0	0	0	0	0	

Step vector representation

h

Step-vector: most efficient CSF encoding

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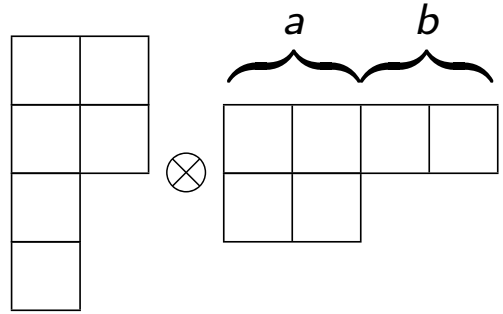
2 bits per spatial orbital
$\rightarrow$ same as Slater Determinants!

UGA Summary

1. Hamiltonian in terms of **generators of U(n)**:

$$\hat{H} = \sum_{ij}^{n} t_{ij} E_{ij} + \frac{1}{2} \sum_{ijkl}^{n} [ij; kl] \left(E_{ij} E_{kl} - \delta_{jk} E_{il} \right)$$

2. **Physical relevant Irreps** of U(n) related to (N, n, S) given by Young shape of U(2)



3. Efficient and unique labeling of **complete basis set** $|\mathbf{d}\rangle$

Hamiltonian Matrix elements

How to calculate:

$$\langle d'|\hat{H}|d\rangle = \sum_{ij}^{n} t_{ij}\langle d'|E_{ij}|d\rangle + \frac{1}{2}\sum_{ijkl}^{n}[ij;kl]\langle d'|(E_{ij}E_{kl} - \delta_{jk}E_{il})|d\rangle$$

E_{ij} moves electron from j to i without changing spin-state.
As opposed to SD more than one possible excitation:

$$E_{ij}|d\rangle = \sum_{k} r_k|d_k\rangle$$

All allowed spin-recouplings between i and j! Eg:

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All allowed spin-recouplings between i and j! Eg:

$$E_{35}|3,1,0,1,2,1,3\rangle = r_1|3,1,1,2,0,1,3\rangle + r_2|3,1,2,1,0,1,3\rangle$$

Graphical UGA in FCIQMC

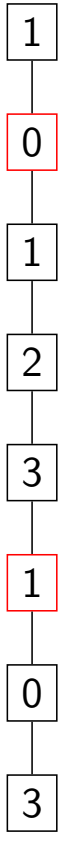
- In FCIQMC we only need **one** possible excitation given $|d\rangle$
- Through Shavitts Graphical Unitary Group Approach:

$$\langle d' | E_{ij} | d \rangle = \prod_{k=i}^{j} W(d'_k, d_k, b_k)$$

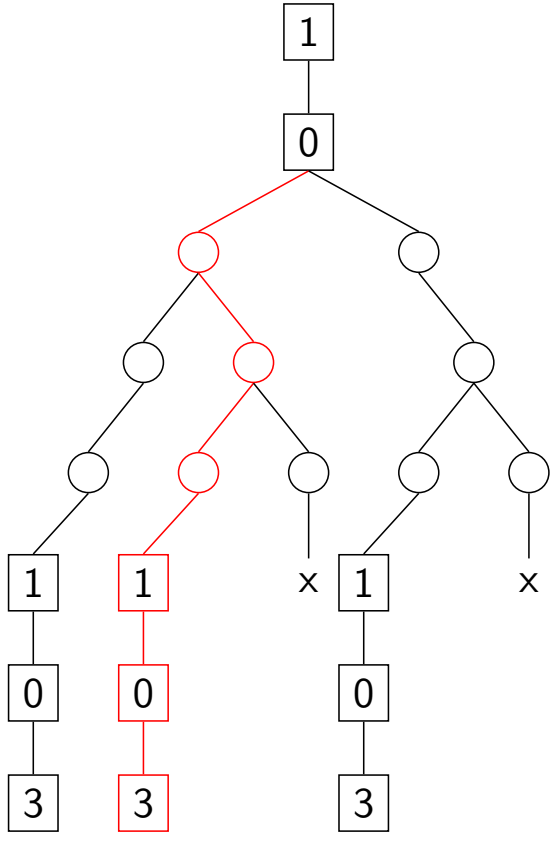
- Loop over $i \rightarrow j$:
- Use a branching diagram and randomly select **one** connected CSF!
- Calculate matrix element on the fly!

GUGA in NECI

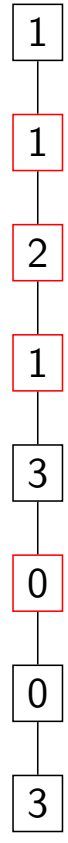
CSF $|m\rangle$



all possible excitations $E_{26}|m\rangle$



specific excitation $|m'\rangle$



Applications

- Scales linear with spatial orbitals $O(n)$
- Slightly slower then determinant based implementation: time per iteration and time-step
- No exponential bottleneck, like previous approaches

Worst case: A lot of open-shell orbitals, while targeting the low-spin eigenstates!

- Real-space Hubbard model for high U up to 20 lattice sites
- AF-reference state with only open-shell orbitals
- Hydrogen-lattice for large atomic distances
- Up to 20 Hydrogen atoms in a minimal basis set

Thank you for your attention!