Efficient Implementation of SU(2) Symmetry

Using the Unitary Group in FCIQMC

W. Dobrautz†, Simon D. Smart and Ali Alavi‡
Max Planck Institute for Solid State Research
email: †werner.dobrautz@gmail.com , ‡A.Alavi@fkf.mpg.de

Introduction and Goals

- Full Configuration Interaction Quantum Monte Carlo (FCIQMC) algorithm[1] is a *projector QMC method*
- Application of $e^{-\tau H}$ yields the ground state of a system in the long-time limit
- Originally formulated in the full anti-symmetric space of Slater Determinants
- Easy usage of translational and lattice symmetries, but until now no application of SU(2) spin symmetry

$\Rightarrow$ Goal: Formulation in $\hat{S}^2$ eigenfunctions via the *Graphical Unitary Group Approach* (GUGA)

In strongly correlated system there are many (near)-degeneracies of eigenstates belonging to different total spin symmetry sectors. In projector type methods, like FCIQMC, efficiency of calculation strongly dependent on energy seperation of low lying eigenstates. $\Rightarrow$ Advantages of $SU(2)$:

- Stabilizing simulation by exclusion of degeneracies of low-lying excitation belonging to different spin-sectors
- Hilbert space size reduction, through further block diagonalization
- Identification of ground state total spin quantum numbers
- Calculation of excited states, through spin-symmetry restrictions

FCIQMC

Projector QMC method in discrete, anti-symmetrized space of Slater Determinants based on the imaginary-time Schrödinger equation:

$$|\Psi_0\rangle = \lim_{\tau\to\infty} \mathrm{e}^{-\tau(H-E_0)}\,|\Psi_T\rangle$$

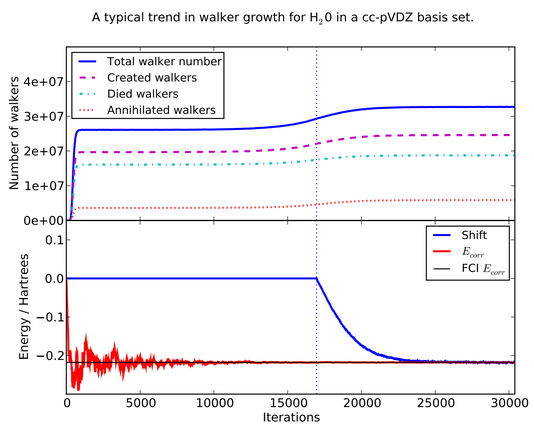
Sample wave function coefficients of $|\Psi\rangle = \sum c_i|D_i\rangle$ by stochastically evolving an ensemble of N_w signed walkers in exponentially large Hilbert space.
Walker population dynamics governed by:

$$c_i^{(n+1)} = \underbrace{\left[1-\tau\left(H_{ii}-E_S\right)\right]c_i^{(n)}}_{\text{death/cloning}} - \underbrace{\tau\sum_{j\neq i} H_{ij}c_j^{(n)}}_{\text{spawning}}$$

Three algorithmic steps:

1. Spawn progeny with probability: $\tau|H_{ij}|$
2. Death or clone with probability: $\tau\left(H_{ii}-E_S\right)$
3. Annihilate oppositely signed walkers on same determinant

Annihilation step crucial to converge to correct fermionic ground state solution. Energy shift E_S tuned to ensure constant walker population gives estimate for ground state energy E_0.
Initiator approximation[2] ensures sign coherent spawning events.

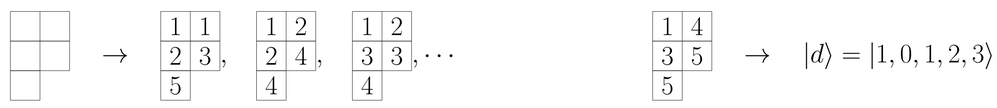


GUGA

The (Graphical) Unitary Group Approach relies on the fact that a spin-preserving, non-relativistic Hamiltonian can be expressed in terms of the *generators* $\hat{E}_{ij}$ of the unitary group $U(n)$:

$$\hat{H} = \sum_{ij}^{n} h_{ij}E_{ij} + \frac{1}{2}\sum_{ijkl}^{n} U_{ijkl}\left(E_{ij}E_{kl} - \delta_{jk}E_{il}\right) \tag{1}$$

with $\hat{E}_{ij} = \hat{a}^\dagger_{i,\uparrow}\hat{a}_{j,\uparrow} + \hat{a}^\dagger_{i,\downarrow}\hat{a}_{j,\downarrow}$ in terms of the usual fermionic creation and annihilation operators and fulfilling the commutation relations of the $U(n)$ generators.
The irreducible representations of $U(n)$, relevant for spin-1/2 systems, can be represented with *Weyl* tableaux with max. two boxes per row. The number of two-box rows a and the number of one-box rows b, determine the electronic configuration. Eg.:

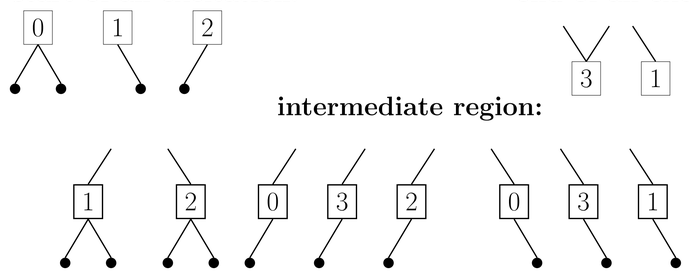


Represents the system with $N_e = 2a + b = 5$ electrons and total spin $S = \frac{b}{2} = 1/2$.
All possible ways to fill up a certain Weyl tableau with tokens, $1, 2, ..., n$, corresponding to spatial orbitals, represent the all spin-adapted states of the Hilbert space of the system.
An efficient way to represent a state is through the *stepvector*[3] **d**, containig information how each orbital gets spin-coupled, which allows efficient storage as bit-strings similar to Slater Determinants :

1. $d_i = 0$: empty orbital i
2. $d_i = 1$: singly couple orbital i, $S + \frac{1}{2}$
3. $d_i = 2$: singly couple orbital i, $S - \frac{1}{2}$
4. $d_i = 3$: doubly occupied orbital i

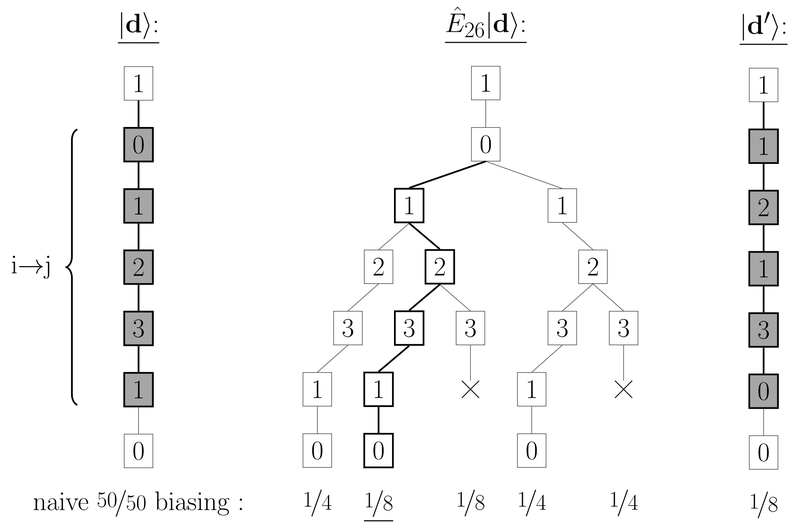
Excitations - diagrammatic representation:

The difference in open orbital number $\Delta b_k = b_k - b'_k$ has to be ± 1 for a single excitation to yield a non-zero overlap matrix element $\langle d'|\hat{E}_{ij}|d\rangle$. This restriction enables a decision-based excitation calculation through a **branching tree:** *Nodes* correspond to stepvector entries **d**, *left going edges* to the $\Delta b = -1$ and *right going edges* to $\Delta b = +1$ branch of an excitation.



Stochastic Excitation Generation

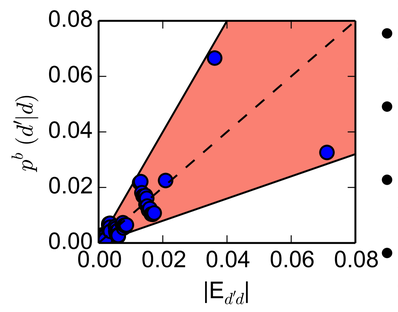
In FCIQMC no knowledge of the full Hilbert space is necessary. In the *spawing step* only **one** of the possible excitations for a given CSF has to be calculated efficiently!
$\rightarrow$ only choose *one* specific path through the branching tree randomly.
For example possible single excitations for: $\hat{E}_{26}|1,0,1,2,3,1,0\rangle$:



A direction change in the branching tree corresponds to different d' values compared to d. Certain d_j values at the end of the excitation only allow specific Δb_j values.

Ratios and Scaling

Relation between probability to choose d' in branching tree $p^b(d'|d)$ and magnitude of generator matrix element $\langle d'|E_{ij}|d\rangle$ using branch weight function biasing for single excitations



- Almost optimal linear ratio $p^b(d'|d) \sim |E_{d'd}|$ for single excitations
- Computational effort scales *linearly* with the number of orbitals, $\sim \mathcal{O}(n)$
- Storage cost per state also scales only *linearly* with number of orbitals
- *On-the-fly* matrix element calculation during excitation generaration
- Double excitation $\hat{E}_{ij}\hat{E}_{kl}|d\rangle$ calculation is more demanding, but also only scales linearly with n

$\Longrightarrow$ GUGA allows efficient $SU(2)$ symmetry implementation in the FCIQMC method!

Matrix Element based Biasing through Branch Weight-Functions

The time step τ in FCIQMC strongly depends on the ratio of the generation probability of state $|d'\rangle$ given $|d\rangle$, $p(d \to d')$, and the magnitude of the off-diagonal Hamiltonian matrix element connecting those states: $|\langle d'|\hat{H}|d\rangle|$.
$p(d'|d)$ is given as a product of an *orbital* and *branching* term and $\langle d'|\hat{H}|d\rangle$ as a sum of products, involving the one- and two-particle integrals and the matrix elements of the generators of the unitary group:

$$p(d'|d) = p^{orb}(d'|d)\cdot p^b(d'|d); \qquad \langle d'|\hat{H}|d\rangle = \sum_{ij} h_{ij}\langle d'|E_{ij}|d\rangle + \frac{1}{2}\sum_{ijkl} U_{ijkl}\langle d'|\left(E_{ij}E_{kl} - \delta_{jk}E_{il}\right)|d\rangle$$

In the GUGA, matrix elements between CSFs can be calculated as a product of terms[4] only depending on the stepvector values d_k and d'_k and the number of open orbitals b_k:

$$\langle d'|\hat{E}_{ij}|d\rangle = \prod_{k\in(i,j)} W(d_k, d'_k, b_k) \quad \text{with} \quad W(d_k,d'_k,b_k) = \begin{cases} \mathcal{O}(1) & \text{for } d_k = d'_k \\ \mathcal{O}(b_k^{-1}) & \text{for } d_k \neq d'_k \end{cases}$$

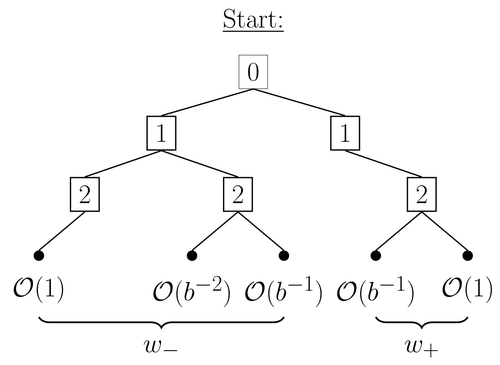
This allows an **on-the-fly** matrix element calculation and allows to ensure an almost optimal linear $p^b(d'|d) \sim |E_{d'd}|$ relation, by taking into account the "probabilistic weight" of different branches in the excitation generation choices, through *branch weight functions* $w_\pm$. Since changing directions in the decision tree yields multiplicative factors of b^{-1} in the matrix element product:

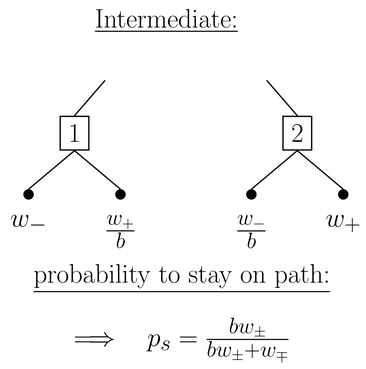
probability to choose $\Delta b = -1$ path at start:

$\Longrightarrow \quad p_- = \frac{w_-}{w_- + w_+}$

$w_- = 1 + \frac{s_-}{b} + \mathcal{O}(b^{-2})$

$w_+ = 1 + \frac{s_+}{b} + \mathcal{O}(b^{-2})$

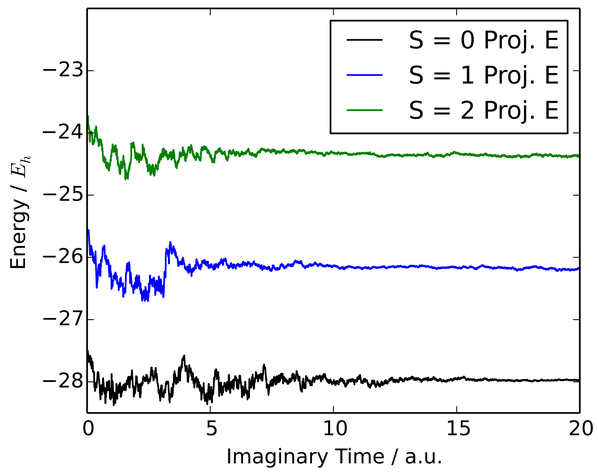




From the start: each branch $\Delta b = \pm 1$ has a single *leaf* corresponding to a matrix element $\mathcal{O}(1)$ and for each following *branching possibilities* $s_\pm$, $d_k = 1$ for $\Delta b = 1$ and $d_k = 2$ for $\Delta b = +1$ an additional *leaf* of $\mathcal{O}(b^{-1})$.

Preliminary Results on the Hubbard Model

The one-band Hubbard model in real-space formulation: $\hat{H} = -t\sum_{<i,j>,\sigma} c^\dagger_{i,\sigma}c_{j,\sigma} + U\sum_i n_{i,\uparrow}n_{i,\downarrow}$



- For strongly correlated electron systems, like the one-band Hubbard model in the intermediate to high interaction regime, the formulation of FCIQMC in spin-adapted eigenfunctions through the GUGA, should improve simulation characteristics.
- Groundstate results for the periodic, 18-site, 18 electron Hubbard model with $U = 1$, using a complete plane-wave basis set with 100000 walkers. Biggest simulation, using $\hat{S}^2$ symmetry, in FCIQMC so far.
- Clear seperation between the spin $S = 0, 1, 2$ groundstates.
- Higher interaction regime, bigger lattice sizes, and influence on simulation performance, topic of further investigation.

References

[1] G. Booth, A. Thom and A. Alavi, J. Chem. Phys. **131**, 054106 (2009)
[2] D. Cleland, G. Booth and A. Alavi, J. Chem. Phys. **132**, 041103 (2010)
[3] J. Paldus, Phys. Rev. A. **14,** 1620 (1976).
[4] I. Shavitt, Int. J. Quantum Chem. Symp., **11:** 131 (1977); Int. J. Quantum Chem. Symp., **12:** 5 (1978).