drudge-gristmill

A Beginners Guide

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Two Modules

Drudge:

- Algebraic Symbolic Manipulator
- Define Hamiltonian, Cluster operators, etc.
- Perform Commutations
- Evaluate expectation values and obtain equations

Gristmill:

- Post-drudge
- Equations obtained from generally scale very badly (CCSD: N^8)
- But if we break multiple tensor contractions into many simple ones, we can improve the scaling (CCSD eventually becomes N^6)

Outline

- Drudge expressions
- Algebras / Libraries
- Basic functions
- Some useful tricks/functions
- Gristmill (?)

Structure (How we understand it)

$$\sum_{i \in O} \sum_{a \in V} f_{a,i} c_a^\dagger c_i + \sum_{i \in O} \sum_{a \in V} f_{i,a} c_i^\dagger c_a$$

Structure (How we understand it)

Expression: $\underbrace{\sum_{i \in O} \sum_{a \in V}}_{\text{Summation}} f_{a,i} \underbrace{c_a^\dagger c_i}_{\text{Operators}} + \sum_{i \in O} \sum_{a \in V} \underbrace{f_{i,a}}_{\text{Tensors}} c_i^\dagger c_a$

Summation

Operators

Tensors

Structure (How drudge understands it)

Term

Tensor: $$\sum_{i\in O}\sum_{a\in V} f_{a,i} c_a^\dagger c_i + \sum_{i\in O}\sum_{a\in V} f_{i,a} c_i^\dagger c_a$$

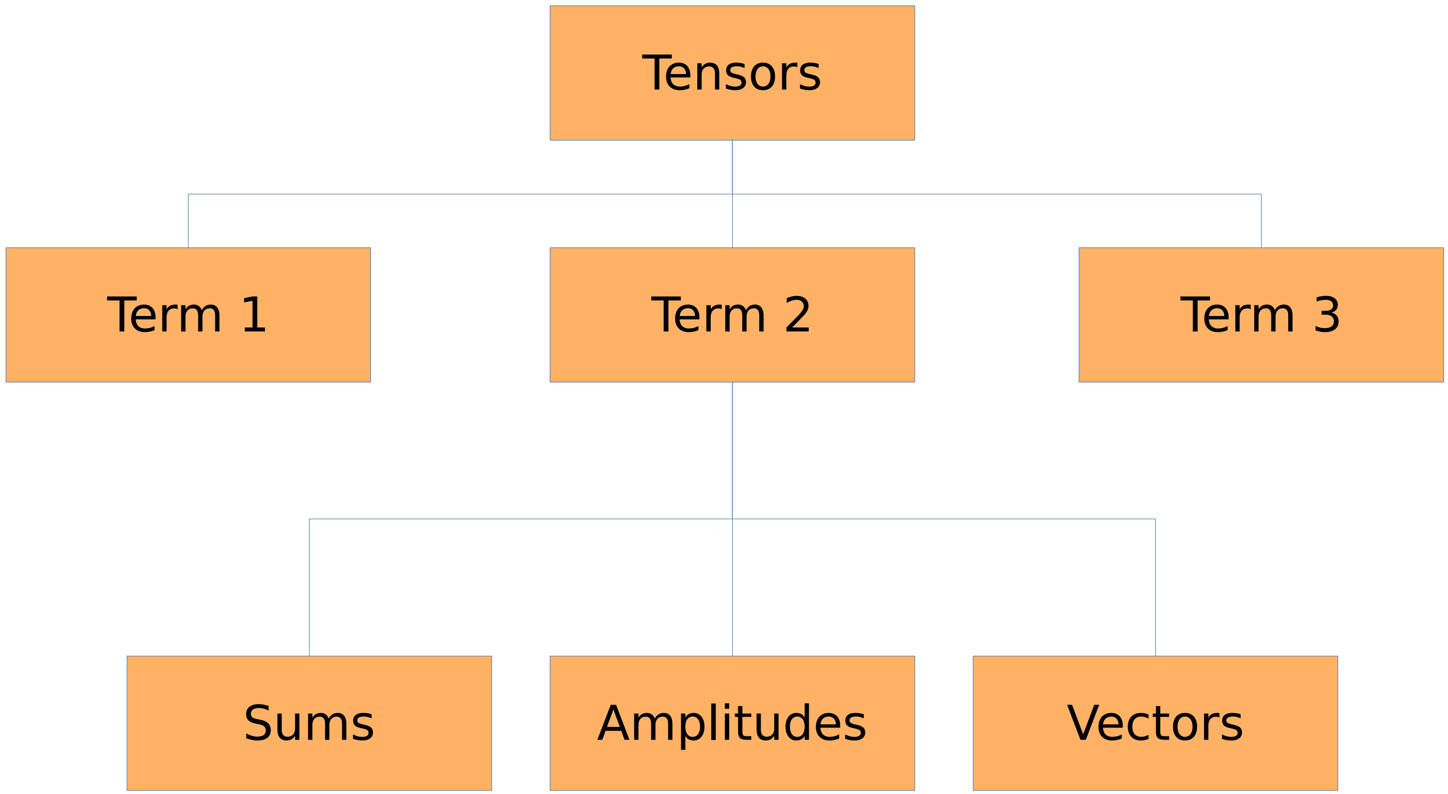
Summation

Vectors

(Base, Index)

Amplitudes

Structure (How drudge understands it)

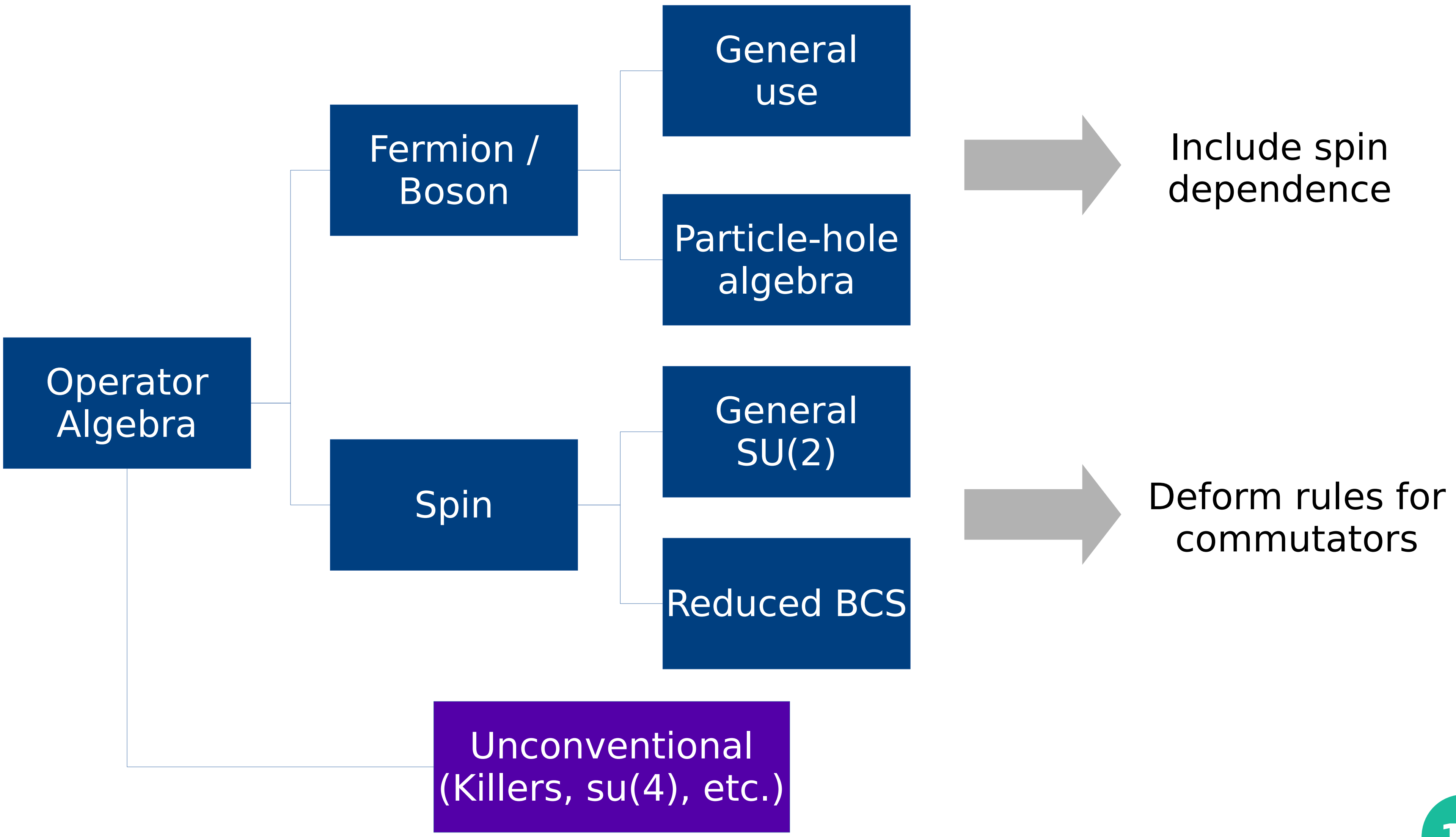


Example

How to Code?

- **Python scripts / Jupyter Notebook**
- **Drudge Script**

Drudge Libraries



Drudge Libraries

1) FockDrudge → generalized framework for both bosons and fermions

2) GenMBDrudge

3) PartHoleDrudge → Introduces notion of particle / hole (or occupied and unoccupied orbitals)

4) SpinOneHalfPartHoleDrudge → when one desires explicit spin-indices

5) SU2LatticeDrudge → SU(2) commutation rules

6) ReducedBCSDrudge → an extension of the SU2LatticeDrudge

How does Drudge work?

Given an expression, say the Hartree-Fock Energy

$$H = \sum_{pq} h_{pq} c_p^\dagger c_q + \frac{1}{4} \sum_{pqrs} u_{pqrs} c_p^\dagger c_q^\dagger c_s c_r \qquad E_{hf} = \langle \Phi | H | \Phi \rangle$$

how would we proceed on paper?

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how would we proceed on paper?

Bring all the terms to their normal ordered form

Normal Ordering

Different kinds of normal ordering – useful for different tasks / applications

1) w.r.t. vacuum

2) w.r.t. fermi-vacuum (particle-hole normal ordering)

3) In spin systems, etc.

Canonical Order

Normal Order ↔ Canonical Order

Operators / Vectors
(non-commutative objects)

Amplitudes – especially with
symmetries;

Basic Functions

- **Commutator**
- **Simplify**
- **Merge**
- **Prepare reports**
- **Symmetry of Indexed Objects**

Examples

Filter and Bind

Gristmill

Say you have the CCSD equations all worked out. In their original form, the scaling is N^8

But these tensor contractions can be optimized by defining suitable intermediates and eventual scaling becomes N^6

Gristmill performs such optimization!

Examples