Automatic derivation of fermionic many-body theories based on general Fermi vacua

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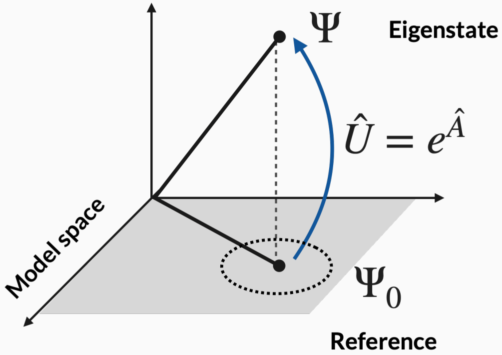
Motivation: Multireference theories

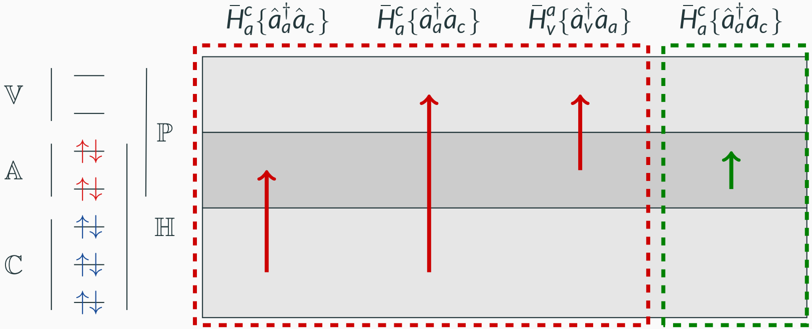
We're interested in developing many-body theories starting from correlated electronic states



Motivation: The Driven Similarity Renormalization Group (DSRG)[1]

$$H \mapsto \bar{H} = e^{-A} H e^{A} = \bar{H}_0 + \sum_{pq} \bar{H}_p^q \{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4} \sum_{pqrs} \bar{H}_{pq}^{rs} \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \dots$$

where $A = T - T^\dagger$ is built from a generalized hole-particle excitation operator T. The components of $\bar{H}$ in red excite model space determinants outside of it and must be removed



[1]Evangelista, F.A. *J. Chem. Phys.* **141**, 054109 (2014).

The generalized normal ordering formalism

To avoid the intruder state problem we solve ***a set of many-body equations*** with an extra source term:

$$\bar{H}^{ab\cdots}_{ij\cdots} = R^{ab\cdots}_{ij\cdots}(s),$$

where the operator $R(s)$ (a regularizer) is derived by matching the DSRG to a low-order perturbative approximation to the SRG

$$R^{ab\cdots}_{ij\cdots}(s) = [\bar{H}^{ab\cdots}_{ij\cdots} + \Delta^{ab\cdots}_{ij\cdots} t^{ab\cdots}_{ij\cdots}] e^{-s(\Delta^{ab\cdots}_{ij\cdots})^2}$$

where the quantity $s \in [0, \infty)$ controls the magnitude of the terms in $\bar{H}^{ab\cdots}_{ij\cdots}$. When $s \to \infty$ we have that $|\bar{H}^{ab\cdots}_{ij\cdots}(s)| \to 0.^*$

Main computational challenge

Generate expressions for normal-ordered operators assuming a general Fermi vacuum Ψ_0.

The generalized normal ordering formalism

Write products of second-quantized operators as

$$\hat{a}^{pq\cdots}_{rs\cdots} = \hat{a}^\dagger_p \hat{a}^\dagger_q \cdots \hat{a}_s \hat{a}_r$$

Consider a ***general reference state*** Ψ_0 with reduced density matrices defined as

$$\gamma^{pq\cdots}_{rs\cdots} = \langle \Psi_0 | \hat{a}^{pq\cdots}_{rs\cdots} | \Psi_0 \rangle$$

Mukherjee[2] defines a normal-ordered operator product $\{\hat{a}^{pq\cdots}_{rs\cdots}\}$ with respect to Ψ_0 to satisfy

Mukherjee's normal ordering condition

$$\langle \Psi_0 | \{\hat{a}^{pq\cdots}_{rs\cdots}\} | \Psi_0 \rangle = 0$$

The operators $\{\hat{a}^{pq\cdots}_{rs\cdots}\}$ represent ***fluctuations*** w.r.t. the reference state.

[2] Mukherjee, D. *Chem. Phys. Lett.* **274**, 561 (1997).

Example: One-particle term

Consider the case of $\hat{a}^p_q = \hat{a}^\dagger_p \hat{a}_q$. Let's assume that we can write $\hat{a}^p_q$ in terms of normal-ordered operators of equal or smaller particle rank:

$$\hat{a}^p_q = \alpha\{\hat{a}^p_q\} + \beta$$

where α, β are scalars. Then by definition

$$\langle\Psi_0|\hat{a}^p_q|\Psi_0\rangle = \alpha \underbrace{\langle\Psi_0|\{\hat{a}^p_q\}|\Psi_0\rangle}_{=0} + \beta$$

and β is given by the one-particle reduced density matrix (1-RDM)

$$\beta = \langle\Psi_0|\hat{a}^p_q|\Psi_0\rangle = \gamma^p_q.$$

When Ψ_0 is the physical vacuum ($|-\rangle$, $\gamma_1 = 0$), then we want $\hat{a}^p_q$ and $\{\hat{a}^p_q\}$ to be identical, so $\alpha = 1$.

$\hat{a}^p_q$ expressed in normal ordered form

$$\hat{a}^p_q = \{\hat{a}^p_q\} + \gamma^p_q \qquad \{\hat{a}^p_q\} = \hat{a}^p_q - \gamma^p_q$$

Wick's theorem

Wick's theorem I

$$
\begin{aligned}
\hat{q}_1\hat{q}_2\cdots ={}& \{\hat{q}_1\hat{q}_2\cdots\} + \sum_{\substack{\text{single}\\\text{pairs}}} \{\hat{q}_1\hat{q}_2\cdots\} \\
&+ \sum_{\substack{\text{double}\\\text{pairs}}} \{\hat{q}_1\hat{q}_2\cdots\} + \sum_{\substack{\text{single}\\\text{4-leg}}} \{\hat{q}_1\hat{q}_2\cdots\} \\
&+ \sum_{\substack{\text{triple}\\\text{pairs}}} \{\hat{q}_1\hat{q}_2\cdots\} + \sum_{\substack{\text{single}\\\text{pairs}}} \sum_{\substack{\text{single}\\\text{4-leg}}} \{\hat{q}_1\hat{q}_2\quad\cdots\} + \ldots.
\end{aligned}
$$

New ***multi-leg contractions*** appear in Wick's theorem.

Wick's theorem

Pairwise contractions yield elements of the one-particle ($\boldsymbol{\gamma}_1$) or one-hole ($\boldsymbol{\eta}_1$) density matrices:

$$\hat{a}_p^\dagger \hat{a}_q = \gamma_q^p \equiv \langle \Psi_0 | \hat{a}_q^p | \Psi_0 \rangle \,,$$
$$\hat{a}_q \hat{a}_p^\dagger = \eta_q^p = \delta_q^p - \gamma_q^p .$$

Multi-legged contractions are elements of the k-body density cumulant ($\boldsymbol{\lambda}_k$)

$$\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r = \lambda_{rs}^{pq} \equiv \gamma_{rs}^{pq} - \gamma_r^p \gamma_s^q + \gamma_s^p \gamma_r^q .$$

For complete-active-space states

$$\boldsymbol{\gamma}_1 = \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\lambda}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \boldsymbol{\eta}_1 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} - \boldsymbol{\lambda}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{1} \end{pmatrix}.$$

Wick's theorem cont'd

A second Wick's theorem applies to products of normal-ordered operators

Wick's theorem II

$$
\begin{aligned}
\{\hat{A}\}\{\hat{B}\}\cdots\{\hat{Z}\} = &\{\hat{A}\hat{B}\cdots\hat{Z}\} + \sum_{\substack{\text{single}\\\text{pairs}}}\{\hat{A}\ \hat{B}\cdots\hat{Z}\} \\
&+ \sum_{\substack{\text{double}\\\text{pairs}}}\{\hat{A}\ \hat{B}\cdots\hat{Z}\} + \sum_{\substack{\text{single}\\\text{4-leg}}}\{\hat{A}\ \hat{B}\cdots\hat{Z}\} \\
&+ \sum_{\substack{\text{triple}\\\text{pairs}}}\{\hat{A}\ \hat{B}\cdots\hat{Z}\} + \ldots.
\end{aligned}
$$

Wick&d

Wick&d

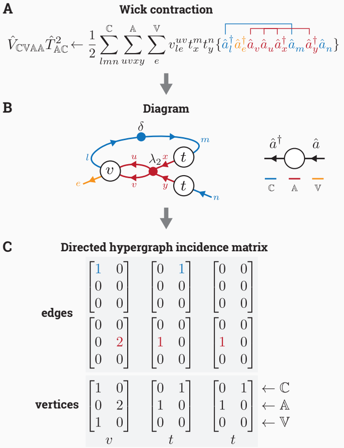
- Implements the algebra of second quantization
- C++ library that implements algebraic and diagrammatic types
- Python bindings generated via the `pybind11` library
- GitHubTest suite (`pytest`), continuous integration (via azure), code coverage

Installing wicked

```
> git clone --recurse-submodules https://github.com/fevangelista/wicked.git
> cd wicked
> python setup.py develop
```

Implementation of Wick's theorem

We represent Wick contractions (A) with directed hypergraphs (B), stored using incidence matrices (C).



Technical aspects

- Orbital spaces
- Representation of operators and contractions
- Generation of contractions
- Canonicalization of contractions
- Translation to equations

Orbital spaces

Partition the spinorbital space $\mathbb{S}$ into subsets:

$$\mathbb{S} = \cup_{k=1}^{s} \mathbb{S}_k.$$

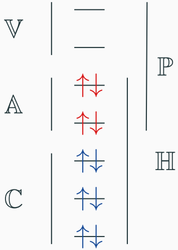
Table 1: Orbital subspaces handled by Wick&d.

Subspace	γ^p_q	η^p_q	$\lambda^{pq\cdots}_{rs\cdots}$
Occupied	δ^p_q	0	0
General	γ^p_q	η^p_q	$\lambda^{pq\cdots}_{rs\cdots}$
Unoccupied	0	δ^p_q	0

Operator notation

In Wick&d operators are represented internally as by a matrix that stores the number of creation/annihilation operators in each space. Suppose we work with a core (double occ

$$\hat{T}_{\mathbb{AC}} = \sum_{m}^{\mathbb{C}} \sum_{u}^{\mathbb{A}} t_{u}^{m} \{ \hat{a}_{u}^{\dagger} \hat{a}_{m} \} \leftrightarrow \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}}_{t} \begin{array}{l} \leftarrow \mathbb{C} \\ \leftarrow \mathbb{A} \\ \leftarrow \mathbb{V} \end{array},$$



Core ($\mathbb{C}$) levels are in blue while active ($\mathbb{A}$) levels are in red.
This is a generalization of the notation used by Kállay and others.

Another example

$$\hat{V}_{\mathbb{C}\mathbb{V}\mathbb{A}\mathbb{A}} = \frac{1}{2}\sum_{m}^{\mathbb{C}}\sum_{uv}^{\mathbb{A}}\sum_{e}^{\mathbb{V}} v_{me}^{uv}\{\hat{a}_m^\dagger \hat{a}_e^\dagger \hat{a}_v \hat{a}_u\} \leftrightarrow \underset{v}{\begin{bmatrix} 1 & 0 \\ 0 & 2 \\ 1 & 0 \end{bmatrix}}$$

- $v_{me}^{uv} = \langle me \| uv \rangle$ is an antisymmetrized two-electron integral.
- The factor $1/2$ accounts for the equivalent indices u and v.

The notation extends to products of operators:

$$\hat{V}_{\mathbb{C}\mathbb{V}\mathbb{A}\mathbb{A}} \frac{1}{2}\hat{T}^2_{\mathbb{A}\mathbb{C}} \leftrightarrow \frac{1}{2} \underset{v}{\begin{bmatrix} 1 & 0 \\ 0 & 2 \\ 1 & 0 \end{bmatrix}} \quad \underset{t}{\begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}} \quad \underset{t}{\begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}}$$

Representation of (elementary) contractions

Elementary contractions are single 2-legged, 4-legged, etc. contractions of operators.
Consider a standard occupied ($\mathbb{O}$)/virtual ($\mathbb{V}$) orbital partitioning:

$$\frac{1}{4}\sum_{ijk}^{\mathbb{O}}\sum_{abc}^{\mathbb{V}} f_k^c t_{ab}^{ij}\{\color{red}{\hat{a}_k^\dagger}\color{black}\hat{a}_c\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_j\,\color{blue}{\hat{a}_i}\color{black}\}$$

Representation of (elementary) contractions

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Consider a standard occupied ($\mathbb{O}$)/virtual ($\mathbb{V}$) orbital partitioning:

$$\frac{1}{4}\sum_{ijk}^{\mathbb{O}}\sum_{abc}^{\mathbb{V}} f_k^c t_{ab}^{ij}\{\hat{a}_k^\dagger \hat{a}_c \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\} \leftrightarrow \begin{array}{cc} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix} \\ f & t \end{array}$$

The boxes on the top indicate ***how many*** operators are contracted, not which ones are contracted.

Equivalent contractions

This is an example of a Wick contraction that connects equivalent second-quantized operators: the contraction $\{\hat{a}_k^\dagger \hat{a}_c \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\}$ is equivalent to $\{\hat{a}_k^\dagger \hat{a}_c \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\}$

$$
\begin{aligned}
&\frac{1}{4}\sum_{ijk}^{\mathbb{O}}\sum_{abc}^{\mathbb{V}} f_k^c t_{ab}^{ij} \{\hat{a}_k^\dagger \hat{a}_c \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\} \\
=&\frac{1}{4}\sum_{ijk}^{\mathbb{O}}\sum_{abc}^{\mathbb{V}} f_k^c t_{ab}^{ji} \{\hat{a}_k^\dagger \hat{a}_c \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_i \hat{a}_j\} \\
=&\frac{1}{4}\sum_{ijk}^{\mathbb{O}}\sum_{abc}^{\mathbb{V}} f_k^c t_{ab}^{ij} \{\hat{a}_k^\dagger \hat{a}_c \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\}
\end{aligned}
$$

Since in the hypergraph representation, equivalent indices are indistinguishable, we account for one of these two equivalent contractions and multiply this term by 2.

Wick&d exploits equivalences to minimize the number of terms generated and facilitate the identification of identical terms.

Composite contractions

In general, Wick's theorem involves multiple elementary contractions. These are represented by stacking rows of elementary contractions (the order is irrelevant)

$$\frac{1}{4}\sum_{ijk}^{\mathbb{O}}\sum_{abc}^{\mathbb{V}} f^{c}_{k} t^{ij}_{ab}\{\hat{a}^{\dagger}_{k}\hat{a}_{c}\hat{a}^{\dagger}_{a}\hat{a}^{\dagger}_{b}\hat{a}_{j}\hat{a}_{i}\} \leftrightarrow \begin{array}{cc} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} & \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \\ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix} \\ f & t \end{array} = \frac{4}{4}\sum_{ij}^{\mathbb{O}}\sum_{ab}^{\mathbb{V}} f^{a}_{i} t^{ij}_{ab}\{\hat{a}^{\dagger}_{b}\hat{a}_{j}\}$$

Generation of contractions. 1) Enumerating elementary contractions

Consider the following term

$$\frac{1}{16}\sum_{c_1c_2c_3c_4}^{\mathbb{C}}\sum_{a_1a_2a_3a_4}^{\mathbb{A}} v^{a_3a_4}_{c_3c_4} t^{c_1c_2}_{a_1a_2}\{\hat{a}^\dagger_{c_3}\hat{a}^\dagger_{c_4}\hat{a}_{a_4}\hat{a}_{a_3}\}\{\hat{a}^\dagger_{a_1}\hat{a}^\dagger_{a_2}\hat{a}_{c_2}\hat{a}_{c_1}\}$$

We can write three elementary contractions ($\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$):

$$\{\hat{a}^\dagger_{\mathbb{C}}\hat{a}^\dagger_{\mathbb{C}}\hat{a}_{\mathbb{A}}\hat{a}_{\mathbb{A}}\}\{\hat{a}^\dagger_{\mathbb{A}}\hat{a}^\dagger_{\mathbb{A}}\hat{a}_{\mathbb{C}}\hat{a}_{\mathbb{C}}\} \leftrightarrow \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = \mathcal{C}_1,$$

Generation of contractions. 1) Enumerating elementary contractions

Consider the following term

$$\frac{1}{16}\sum_{c_1c_2c_3c_4}^{\mathbb{C}}\sum_{a_1a_2a_3a_4}^{\mathbb{A}} v_{c_3c_4}^{a_3a_4} t_{a_1a_2}^{c_1c_2}\{\hat{a}_{c_3}^{\dagger}\hat{a}_{c_4}^{\dagger}\hat{a}_{a_4}\hat{a}_{a_3}\}\{\hat{a}_{a_1}^{\dagger}\hat{a}_{a_2}^{\dagger}\hat{a}_{c_2}\hat{a}_{c_1}\}$$

We can write three elementary contractions ($\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$):

$$\{\hat{a}_{\mathbb{C}}^{\dagger}\hat{a}_{\mathbb{C}}^{\dagger}\hat{a}_{\mathbb{A}}\hat{a}_{\mathbb{A}}\}\{\hat{a}_{\mathbb{A}}^{\dagger}\hat{a}_{\mathbb{A}}^{\dagger}\hat{a}_{\mathbb{C}}\hat{a}_{\mathbb{C}}\} \leftrightarrow \begin{bmatrix}1 & 0\\0 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\0 & 0\\0 & 0\end{bmatrix} = \mathcal{C}_1,$$

$$\{\hat{a}_{\mathbb{C}}^{\dagger}\hat{a}_{\mathbb{C}}^{\dagger}\hat{a}_{\mathbb{A}}\hat{a}_{\mathbb{A}}\}\{\hat{a}_{\mathbb{A}}^{\dagger}\hat{a}_{\mathbb{A}}^{\dagger}\hat{a}_{\mathbb{C}}\hat{a}_{\mathbb{C}}\} \leftrightarrow \begin{bmatrix}0 & 0\\0 & 1\\0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\1 & 0\\0 & 0\end{bmatrix} = \mathcal{C}_2,$$

Generation of contractions. 1) Enumerating elementary contractions

Consider the following term

$$\frac{1}{16}\sum_{c_1c_2c_3c_4}^{\mathbb{C}}\sum_{a_1a_2a_3a_4}^{\mathbb{A}} v^{a_3a_4}_{c_3c_4}\, t^{c_1c_2}_{a_1a_2}\{\hat{a}^\dagger_{c_3}\hat{a}^\dagger_{c_4}\hat{a}_{a_4}\hat{a}_{a_3}\}\{\hat{a}^\dagger_{a_1}\hat{a}^\dagger_{a_2}\hat{a}_{c_2}\hat{a}_{c_1}\}$$

We can write three elementary contractions ($\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$):

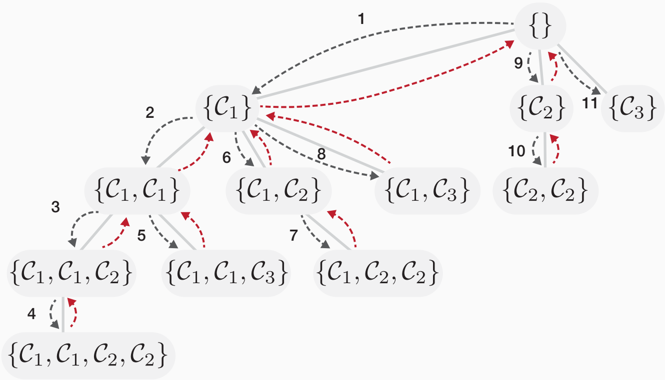
$$\{\hat{a}^\dagger_{\mathbb{C}}\hat{a}^\dagger_{\mathbb{C}}\hat{a}_{\mathbb{A}}\hat{a}_{\mathbb{A}}\}\{\hat{a}^\dagger_{\mathbb{A}}\hat{a}^\dagger_{\mathbb{A}}\hat{a}_{\mathbb{C}}\hat{a}_{\mathbb{C}}\} \leftrightarrow \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = \mathcal{C}_1,$$

$$\{\hat{a}^\dagger_{\mathbb{C}}\hat{a}^\dagger_{\mathbb{C}}\hat{a}_{\mathbb{A}}\hat{a}_{\mathbb{A}}\}\{\hat{a}^\dagger_{\mathbb{A}}\hat{a}^\dagger_{\mathbb{A}}\hat{a}_{\mathbb{C}}\hat{a}_{\mathbb{C}}\} \leftrightarrow \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \end{bmatrix} = \mathcal{C}_2,$$

$$\{\hat{a}^\dagger_{\mathbb{C}}\hat{a}^\dagger_{\mathbb{C}}\hat{a}_{\mathbb{A}}\hat{a}_{\mathbb{A}}\}\{\hat{a}^\dagger_{\mathbb{A}}\hat{a}^\dagger_{\mathbb{A}}\hat{a}_{\mathbb{C}}\hat{a}_{\mathbb{C}}\} \leftrightarrow \begin{bmatrix} 0 & 0 \\ 0 & 2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 2 & 0 \\ 0 & 0 \end{bmatrix} = \mathcal{C}_3.$$

Generation of contractions. 2) Enumerating composite contractions

All the unique composite contractions are generated by backtracking



Composite contractions

$\{\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1,\mathcal{C}_1\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1,\mathcal{C}_1,\mathcal{C}_2\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1,\mathcal{C}_1,\mathcal{C}_2,\mathcal{C}_2\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1,\mathcal{C}_1,\mathcal{C}_3\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1,\mathcal{C}_2\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1,\mathcal{C}_2,\mathcal{C}_2\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_1,\mathcal{C}_3\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_2\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_2,\mathcal{C}_2\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$
$\{\mathcal{C}_3\}$	$\{\hat a^\dagger_{\mathbb{C}}\hat a^\dagger_{\mathbb{C}}\hat a_{\mathbb{A}}\hat a_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a^\dagger_{\mathbb{A}}\hat a_{\mathbb{C}}\hat a_{\mathbb{C}}\}$

The backtracking algorithm produces diagrams with distinct connectivity. Nevertheless, it is still possible to generate isomorphic diagrams that yield equivalent algebraic terms.

Consider the term $\langle\Psi_0|[\hat{V}_{\mathbb{AAAA}}, \hat{T}_{\mathbb{AAAA}}]|\Psi_0\rangle = 0$

$$\hat{V}_{\mathbb{AAAA}}\hat{T}_{\mathbb{AAAA}} \leftarrow \frac{1}{16} v^{uv}_{st} t^{yz}_{wx}\{\hat{a}^\dagger_s \hat{a}^\dagger_t \hat{a}_v \hat{a}_u \hat{a}^\dagger_w \hat{a}^\dagger_x \hat{a}_z \hat{a}_y\} \leftrightarrow \begin{array}{cc} \begin{bmatrix}2 & 0\end{bmatrix} & \begin{bmatrix}0 & 2\end{bmatrix} \\ \begin{bmatrix}0 & 2\end{bmatrix} & \begin{bmatrix}2 & 0\end{bmatrix} \\ \begin{bmatrix}2 & 2\end{bmatrix} & \begin{bmatrix}2 & 2\end{bmatrix} \\ v & t \end{array} .$$

$$\hat{T}_{\mathbb{AAAA}}\hat{V}_{\mathbb{AAAA}} \leftarrow \frac{1}{16} v^{uv}_{st} t^{yz}_{wx}\{\hat{a}^\dagger_w \hat{a}^\dagger_x \hat{a}_z \hat{a}_y \hat{a}^\dagger_s \hat{a}^\dagger_t \hat{a}_v \hat{a}_u\} \leftrightarrow \begin{array}{cc} \begin{bmatrix}2 & 0\end{bmatrix} & \begin{bmatrix}0 & 2\end{bmatrix} \\ \begin{bmatrix}0 & 2\end{bmatrix} & \begin{bmatrix}2 & 0\end{bmatrix} \\ \begin{bmatrix}2 & 2\end{bmatrix} & \begin{bmatrix}2 & 2\end{bmatrix} \\ t & v \end{array} .$$

These are identical terms but may have ***different algebraic expressions***. We use ***early canonicalization*** to cancel these out.

Hypergraph canonicalization

The incidence matrix $\mathcal{W}$ for a contraction can be written as

$$\mathcal{W} = \begin{array}{cc} \begin{bmatrix} \mathbf{C}_{1L} & \mathbf{C}_{2L} & \cdots & \mathbf{C}_{KL} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{C}_{11} & \mathbf{C}_{21} & \cdots & \mathbf{C}_{K1} \\ \mathbf{N}_1 & \mathbf{N}_2 & \cdots & \mathbf{N}_K \\ \omega_1 & \omega_2 & \cdots & \omega_K \end{bmatrix} & L \text{ rows} \\ K \text{ columns} & \end{array}$$

We define the ***canonical*** form as the ***minimal element among all the valid permutations***, where lexicographic ordering of the entries of $\mathcal{W}$ are used to define an ordering among the incidence matrices ($\mathcal{W} < \mathcal{W}'$).

In practice, we may have to test up to $K!L!$ permutations of the entries of $\mathcal{W}$. ***Is this optimal?***

Conversion to algebraic expressions

Consider, for example, the following contraction

$$\{\mathcal{C}_1, \mathcal{C}_1\} \to \{\hat{a}^\dagger_{\mathbb{C}} \hat{a}^\dagger_{\mathbb{C}} \hat{a}_{\mathbb{A}} \hat{a}_{\mathbb{A}} \hat{a}^\dagger_{\mathbb{A}} \hat{a}^\dagger_{\mathbb{A}} \hat{a}_{\mathbb{C}} \hat{a}_{\mathbb{C}}\}.$$

Assign distinct indices to the operators (preserving order)

$$\frac{1}{16} v^{a_2 a_1}_{c_1 c_2} t^{c_4 c_3}_{a_3 a_4} \{\hat{a}^\dagger_{c_1} \hat{a}^\dagger_{c_2} \hat{a}_{a_1} \hat{a}_{a_2} \hat{a}^\dagger_{a_3} \hat{a}^\dagger_{a_4} \hat{a}_{c_3} \hat{a}_{c_4}\}.$$

Next, reorder this term keeping contracted operators adjacent, keeping track of sign factors

$$\frac{1}{16} v^{a_2 a_1}_{c_1 c_2} t^{c_4 c_3}_{a_3 a_4} \underbrace{\hat{a}^\dagger_{c_1} \hat{a}_{c_4}}_{\delta_{c_1 c_4}} \underbrace{\hat{a}^\dagger_{c_2} \hat{a}_{c_3}}_{\delta_{c_2 c_3}} \{\hat{a}_{a_1} \hat{a}_{a_2} \hat{a}^\dagger_{a_3} \hat{a}^\dagger_{a_4}\}.$$

Simplify the δ's and multiply by ***combinatorial*** factors (here 2 for the equivalent contractions)

$$\frac{1}{8} \sum_{c_1 c_2}^{\mathbb{C}} \sum_{a_1 a_2 a_3 a_4}^{\mathbb{A}} v^{a_3 a_4}_{c_1 c_2} t^{c_1 c_2}_{a_1 a_2} \{\hat{a}^\dagger_{a_1} \hat{a}^\dagger_{a_2} \hat{a}_{a_4} \hat{a}_{a_3}\}.$$

How is Wick&d implemented?

The example below shows the evaluation of the CC term $\langle \Phi | \hat{F}_{ov} \hat{T}_1 | \Phi \rangle$ in Python and the corresponding C++ classes

```
class WickTheorem
```

```
class OperatorExpression
```

1
```
wt = w.WickTheorem()
```

2
```
Fov = w.op('f',['o+ v'])
T1 = w.op('f',['v+ o'])
```

3
```
expr = wt.contract(Fov @ T1,0,0)
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In this code we:

1. Make a `WickTheorem` object
2. Make the `Fov` and `T1` operators
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class Expression
```

In this code we:

1. Make a `WickTheorem` object
2. Make the `Fov` and `T1` operators
3. Evaluate the contraction

The `Expression` object relies on several underlying classes:

$$\underbrace{\underbrace{h^q_p \hat{a}^\dagger_p \hat{a}_q}_{\text{Term}} + \underbrace{\frac{1}{4}\underbrace{v^{rs}_{pq}\hat{a}^\dagger_p \hat{a}^\dagger_q \hat{a}_s \hat{a}_r}_{\text{SymbolicTerm}}}_{\text{Term}}}_{\text{Expression}}$$

The split `Term`/`SymbolicTerm` facilitates the grouping of terms in `Expression` (stored as a `SymbolicTerm` $\to$ `scalar_t` map).

What can Wick&d do?

- Evaluate vacuum expectation values with respect to a general Ψ_0.
- Put operator in normal-ordered form.
- Translate algebraic equations into tensor contractions (not optimized).

Arbitrary-order CC equations

In CC theory we are interested in computing the residuals $r^{ij\cdots}_{ab\cdots}$

$$r^{ij\cdots}_{ab\cdots} = \langle \Phi | \{\hat{a}^{ij\cdots}_{ab\cdots}\} \bar{H} | \Phi \rangle$$

Strategy I

Compute

$$Z(\omega) = \frac{1}{(k!)^2} \sum_{ij\cdots} \sum_{ab\cdots} \omega^{ab\cdots}_{ij\cdots} \langle \Phi | \{\hat{a}^{ij\cdots}_{ab\cdots}\} \bar{H} | \Phi \rangle = \langle \Phi | \hat{\Omega} \bar{H} | \Phi \rangle$$

and obtain the residuals as

$$r^{ij\cdots}_{ab\cdots} = \frac{\partial}{\partial \omega^{ab\cdots}_{ij\cdots}} Z(\omega)$$

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$$r^{ij\cdots}_{ab\cdots} = \langle\Phi|\{\hat{a}^{ij\cdots}_{ab\cdots}\}\bar{H}|\Phi\rangle$$

Strategy II

Compute

$$\bar{H} = E_0 + \sum_{pq} \bar{H}^{q}_{p}\{\hat{a}^{p}_{q}\} + \frac{1}{4}\sum_{pqrs} \bar{H}^{rs}_{pq}\{\hat{a}^{pq}_{rs}\} + \ldots,$$

and obtain (via Wick's theorem)

$$r^{ij\cdots}_{ab\cdots} = (k!)^2 \mathcal{A}_{ij\cdots}\mathcal{A}_{ab\cdots}\bar{H}^{ij\cdots}_{ab\cdots}$$

Arbitrary-order CC equations

Table 2: Evaluation of the coupled cluster residual equations with Wick&d. Execution time and the number of unique terms contributing to the residual equations at a given particle-hole excitation level.

Theory	Time	Diagrams per excitation level								
	(s)	0	1	2	3	4	5	6	7	8
CCSD	0.1	3	14	31						
CCSDT	0.7	3	15	37	47					
CCSDTQ	2.4	3	15	38	53	74				
CCSDTQP	6.3	3	15	38	54	80	99			
CCSDTQPH	13.8	3	15	38	54	81	105	135		
CCSDTQPH7	26.0	3	15	38	54	81	106	141	169	
CCSDTQPH78	45.4	3	15	38	54	81	106	142	175	215

Fun fact: Getting the high-order terms right requires using arbitrary precision integers.

Live demo!