

July 30, 2018

## In-Medium SRG

We saw in the 2-level system example that the SRG can be used to obtain the eigenvalues of a bound system. We also saw that, when we use a Fock space formalism the SRG generates many-body terms in the Hamiltonian. If we neglect 3,4,5... body terms, then our transformation is no longer unitary. On the other hand, keeping them explicitly is computationally painful for interesting systems.

Our SRG-evolved Hamiltonian will schematically look like

$$H(s) = \sum_{pq} H^{(1)}_{pq} a_p^+ a_q + \frac{1}{4} \sum_{pqrs} H^{(2)}_{pqrs} a_p^+ a_q^+ a_s a_r + \frac{1}{(3!)^2} \sum_{pqrs tu} H^{(3)}_{pqrs tu} a_p^+ a_q^+ a_r^+ a_u a_t a_s \\ + \frac{1}{(4!)^2} \sum H^{(4)} a^+ a^+ a^+ a^+ a a a a + \dots$$

If the size of the induced many-body forces remains small, i.e.  $H^{(4)} \ll H^{(3)} \ll H^{(2)}$ , then we may be justified in neglecting them. Unfortunately, in nuclear physics, the induced forces aren't small enough for the desired accuracy.

But we can improve things by using normal ordering. The thing that really impacts our final result is the expectation value, e.g.

$$\langle 4 | H^{(4)} a^+ a^+ a^+ a^+ a a a a | 4 \rangle$$

We can make this contribution small by either

making  $H^{(4)}$  small, or by making  $\langle 4|a^\dagger a^\dagger a^\dagger a^\dagger|4\rangle$  small.

To achieve this, let's define a normal ordered string of creation and annihilation operators as

$$\langle \Phi | \{a^\dagger a^\dagger \dots a a\} | \Phi \rangle = 0.$$

Here,  $|\Phi\rangle$  is our "reference state" which dictates what ordering is "normal". For the special case where our reference is the vacuum, i.e.  $|\Phi\rangle = |0\rangle$ , then normal ordering is defined as

$$\langle 0 | \{a^\dagger a^\dagger \dots a a\} | 0 \rangle = 0. \quad (\text{vacuum normal-ordering})$$

To ensure this, we can move all the  $a^\dagger$ 's to the left and all the  $a$ 's to the right. Since  $a|0\rangle = 0$ , we satisfy the above requirement. To be clear, any ordering with an  $a$  on the right or an  $a^\dagger$  on the left will satisfy the requirement. Evidently, the normal order is not unique.

Before reviewing how normal ordering works for a reference other than the true vacuum, I want to illustrate how this will help us. If we write our operator in terms of normal ordered strings of creation and annihilation operators,

$$H = E_0 + \sum_{pq} H_{pq}^{[1]} \{a_p^\dagger a_q\} + \frac{1}{(2!)^2} \sum_{pqrs} H_{pqrs}^{[2]} \{a_p^\dagger a_q^\dagger a_s a_r\} + \frac{1}{(3!)^2} \sum H^{[3]} \{a^\dagger a^\dagger a^\dagger a a a\} + \dots$$

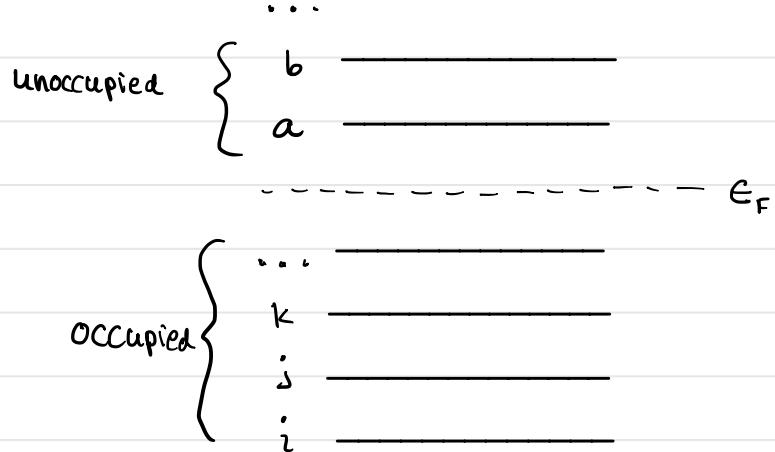
and if we choose a reference state which approximates the exact wave function, i.e.  $|\Phi\rangle \approx |4\rangle$ , then

$$\langle 4 | H^{[4]} \{ a^+ a^- a^+ a^- a a a a \} | 4 \rangle \approx \langle \Phi | H^{[4]} \{ a^+ a^- a^+ a^- a a a a \} | \Phi \rangle = 0.$$

This clearly improves the truncation of keeping only up to 2 or 3-body terms. Even if  $h^{(n)}$  is nonzero, the fact that we use normal ordered operators kills off these terms — so long as  $|\Phi\rangle \approx |4\rangle$ .

Now, back to normal ordering with a non-vacuum reference state. Our state consists of some number of occupied orbits. For example, these could be the lowest few orbits from a Hartree-Fock calculation.

$$|\Phi\rangle = |ijk\dots\rangle = a_i^+ a_j^+ a_k^+ \dots |0\rangle$$



As in previous discussions, we use  $ijk\dots$  to indicate occupied levels and  $abc$  to indicate unoccupied levels.

So now what is the normal order for the operator string  $a_i^+ a_i$ ? Since orbit  $i$  is occupied in  $|\Phi\rangle$ , we have

$$\langle \Phi | a_i^+ a_i | \Phi \rangle = 1 \neq 0.$$

If we try the other ordering,

$$\langle \Phi | a_i a_i^+ | \Phi \rangle = 0$$

because we are trying to add a particle to a level that is already occupied.

So

$$\{a_i^+ a_i\} = -a_i a_i^+$$

(The minus sign came from commuting the operators.)

Creation/annihilation operators for the unoccupied levels behave in the same way as for the vacuum reference case:

$$\langle \Phi | a_a^+ a_a | \Phi \rangle = 0 , \quad \langle \Phi | a_a a_a^+ | \Phi \rangle = 1$$

$$\{a_a^+ a_a\} = a_a^+ a_a.$$

This makes some sense, because in the vacuum case all levels are unoccupied.

## Wick's Theorem

To express some arbitrary string of creation/annihilation operators in terms of normal ordered strings, we use Wick's theorem. To state the theorem, I use  $\alpha_p$  to indicate either  $a_p^*$  or  $a_p$ .

Wick's theorem states:

$$\begin{aligned} \alpha_p \alpha_q \alpha_r \dots \alpha_z &= \{ \alpha_p \alpha_q \alpha_r \dots \alpha_z \} + \{ \overline{\alpha_p} \overline{\alpha_q} \alpha_r \dots \alpha_z \} \\ &+ \{ \overline{\alpha_p} \alpha_q \overline{\alpha_r} \dots \alpha_z \} + (\text{all single contractions}) \\ &+ \{ \overline{\alpha_p} \overline{\alpha_q} \overline{\alpha_r} \dots \alpha_z \} + \{ \overline{\alpha_p} \overline{\alpha_q} \overline{\alpha_r} \dots \overline{\alpha_z} \} + (\text{all double contractions}) \\ &+ \{ \overline{\alpha_p} \overline{\alpha_q} \overline{\alpha_r} \dots \overline{\alpha_z} \} + (\text{all triple contractions}) \\ &+ \dots \end{aligned}$$

Here, we have introduced the concept of a contraction of two operators. The contraction is a plain old number (i.e. not an operator) which may be defined by assuming Wick's theorem holds for a string of two operators.

$$\alpha_p \alpha_q = \{ \alpha_p \alpha_q \} + \{ \overline{\alpha_p} \overline{\alpha_q} \}.$$

Sandwiching this between the reference state yields

$$\langle \Phi | \alpha_p \alpha_q | \Phi \rangle = \overline{\alpha_p} \overline{\alpha_q}.$$

Moving back from the generic  $\alpha_p$  to  $a_p^+$  and  $a_p$ , we can evaluate the various contractions.

$$\overline{a_p^+ a_q} = \langle \Phi | a_p^+ a_q | \Phi \rangle = \rho_{pq} = \delta_{pq} n_p$$

for an uncorrelated reference state

The one-body density matrix  $\rho_{pq}$  is just the expectation value of  $a_p^+ a_q$  in the reference state. If our reference is a single Slater determinant, then  $\rho_{pq} = 0$  unless  $p=q$  and  $p$  is occupied in  $|\Phi\rangle$ . The occupation number  $n_p$  is

$$n_p = \begin{cases} 1 & p \text{ occupied} \\ 0 & p \text{ unoccupied} \end{cases}.$$

$$\overline{a_p^+ a_q^+} = \langle \Phi | a_p^+ a_q^+ | \Phi \rangle = 0.$$

$$\overline{a_p a_q} = \langle \Phi | a_p a_q | \Phi \rangle = 0.$$

And finally,

$$\overline{a_p a_q^+} = \langle \Phi | a_p a_q^+ | \Phi \rangle = \bar{\rho}_{pq} = \delta_{pq} \bar{n}_p = \delta_{pq} (1 - n_p)$$

↑  
uncorrelated reference

where  $\bar{\rho}_{pq}$  is the one-body hole density.

With Wick's theorem and our contractions in hand, we can express our operators in normal ordered form.

$$H = \sum_{pq} t_{pq} a_p^+ a_q + \frac{1}{(2!)^2} \sum_{pqrs} V_{pqrs} a_p^+ a_q^+ a_s a_r + \frac{1}{(3!)^2} \sum_{\substack{pqrs \\ stu}} V^{(3)}_{pqrsstu} a_p^+ a_q^+ a_r^+ a_u a_t a_s + \dots$$

Applying Wick's theorem,

$$\bullet a_p^+ a_q = \{a_p^+ a_q\} + \overbrace{a_p^+ a_q}^{\square}$$

$$= \{a_p^+ a_q\} + \delta_{pq} n_p.$$

$$\bullet a_p^+ a_q^+ a_s a_r = \{a_p^+ a_q^+ a_s a_r\} + \{a_p^+ \overbrace{a_q^+ a_s a_r}^{\square}\} + \{a_p^+ \overbrace{a_q^+ a_s a_r}^{\square}\} + \{a_p^+ \overbrace{a_q^+ a_s a_r}^{\square}\} + \{a_p^+ \overbrace{a_q^+ a_s a_r}^{\square}\}$$

$$+ \{a_p^+ \overbrace{a_q^+ a_s a_r}^{\square}\} + \{a_p^+ \overbrace{a_q^+ a_s a_r}^{\square}\}$$

$$= \{a_p^+ a_q^+ a_s a_r\} + \delta_{qs} n_q \{a_p^+ a_r\} + \delta_{pr} n_p \{a_q^+ a_s\} - \delta_{qr} n_q \{a_p^+ a_s\} - \delta_{ps} n_p \{a_q^+ a_r\}$$

$$+ \delta_{qs} \delta_{pr} n_p n_q - \delta_{ps} \delta_{qr} n_p n_q.$$

The application of Wick's theorem to the 3-body operator is left as an exercise.

The normal-ordered form of H may be written as

$$H = E_0 + \sum_{pq} f_{pq} \{a_p^+ a_q\} + \frac{1}{(2!)^2} \sum_{pqrs} \Gamma_{pqrs} \{a_p^+ a_q^+ a_s a_r\} + \frac{1}{(3!)^2} \sum_{\substack{pqrs \\ stu}} W_{pqrsstu} \{a_p^+ a_q^+ a_r^+ a_u a_t a_s\}$$

Collecting coefficients and relabeling summed-over indices when convenient, we obtain the following relationship between the reference normal-ordered and vacuum normal-ordered coefficients.

3-body piece in full glory, (for those with a strong stomach)

$$E_0 = \sum_i n_i t_{ii} + \frac{1}{2} \sum_{ij} n_i n_j V_{ijij} + \frac{1}{6} \sum_{ijk} n_i n_j n_k V_{ijkijk}^{(3)}$$

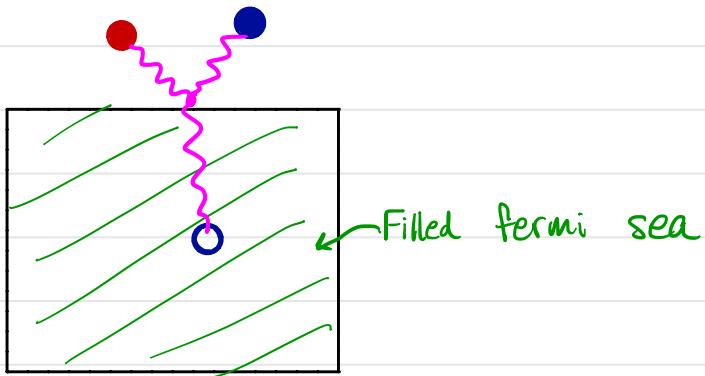
$$f_{pq} = t_{pq} + \sum_i n_i V_{piqi} + \frac{1}{2} \sum_{ij} n_i n_j V_{pijqij}^{(3)}$$

$$\Gamma_{pqrs} = V_{pqrs} + \sum_i n_i V_{pqisri}^{(3)}$$

$$W_{pqrsiu} = V_{pqrsiu}^{(3)} .$$

Before moving on to the IMSRG flow equations, let's look at what the normal ordering has bought us. The effects of the 3-body potential are now spread across  $E_0$ ,  $f$ ,  $\Gamma$ , and  $W$ . By discarding  $W$ , we throw away less than if we had just discarded  $V^{(3)}$ . Note that we pay for this with a loss of generality - our Hamiltonian is now optimized for a specific reference state. Also, the reference breaks Galilean invariance and so we cannot ignore the center of mass.

Pictorially, the idea looks something like this:



We obtain an effective 2-body interaction by summing the third leg of the 3-body interaction over the occupied states in the fermi sea.

## IMSRG Flow Equations

We now express  $H$  and  $\eta$  as Fock-space operators in normal-ordered form:

$$H = E_0 + \sum_{pq} f_{pq} \{a_p^\dagger a_q\} + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} \{a_p^\dagger a_q^\dagger a_s a_r\} + \dots$$

$$\eta = \sum_{pq} \eta_{pq} \{a_p^\dagger a_q\} + \frac{1}{4} \sum_{pqrs} \eta_{pqrs} \{a_p^\dagger a_q^\dagger a_s a_r\} + \dots$$

Our task, then, is to evaluate the commutator in this form. One can directly apply Wick's theorem, but this quickly gets tedious and repetitive. It's slightly less tedious, and more physically illuminating, to use diagrams. Deriving the full expression is still a bit onerous, so we'll do one term and quote the result for the rest.

## Hugenholtz diagrams

We'll use what are called Hugenholtz diagrams to begin with. They look like this

$$\eta = \sum_{pq} \text{(Diagram 1)} + \sum_{pqrs} \text{(Diagram 2)}$$

These diagrams take advantage of the antisymmetry of indices, i.e.  $\eta_{pqrs} = -\eta_{qprs}$  (note, this is distinct from the antihermiticity), and significantly reduce the number of diagrams required. However, to interpret a diagram and

turn it into a formula, we need to expand it into a Goldstone diagram, which stretches out the interaction vertex

$$\begin{array}{ccc}
 \text{Hugenholtz} & \xrightarrow{\quad} & \text{Goldstone} \\
 \begin{array}{c} p \\ \diagup \quad \diagdown \\ \text{H} \\ \diagdown \quad \diagup \\ r \quad s \end{array} & & \begin{array}{c} p \\ \diagup \quad \diagdown \\ \text{H} \\ \diagdown \quad \diagup \\ r \quad s \end{array} = \langle pq | H | rs \rangle
 \end{array}$$

There are multiple ways to expand a Hugenholtz diagram to a Goldstone diagram - we just need to pick one.

To interpret a diagram, we have the following rules

- 1) Obtain a phase factor  $(-)^{l-h}$ , with  $l = \# \text{ of loops}$ , and  $h = \# \text{ of hole lines}$ .
- 2) Obtain a symmetry factor  $\frac{1}{N!}$  when  $N$  equivalent lines connect two nodes in a Hugenholtz diagram.
- 3) Expand the Hugenholtz diagram to an equivalent Goldstone diagram. Hugenholtz and Goldstone diagrams for a 1-body operator are identical.
- 4) Sum over internal lines, including a factor  $n$  for hole lines and  $\bar{n}$  for particle lines.
- 5) Enforce antisymmetry (as necessary) by multiplying by, e.g.  $\frac{1}{2}(1-P_{pq})$ .

As an example, we will calculate  $[\eta^{[2]}, H^{[2]}]^{[1]}$ , that is, the contribution to the 1-body piece of the commutator due to the 2-body piece of  $\eta$  and the 2-body piece of  $H$ .

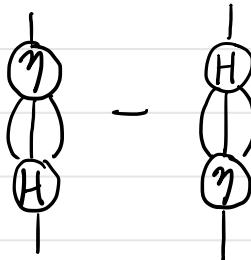
Explicitly, the commutator will be an operator which we also express as a Fock-space operator, let's call it  $C = [\eta, H]$ , so

$$C = \sum_{pq} C_{pq} \{a_p^\dagger a_q\} + \frac{1}{4} \sum_{pqrs} C_{pqrs} \{a_p^\dagger a_q^\dagger a_s a_r\}$$

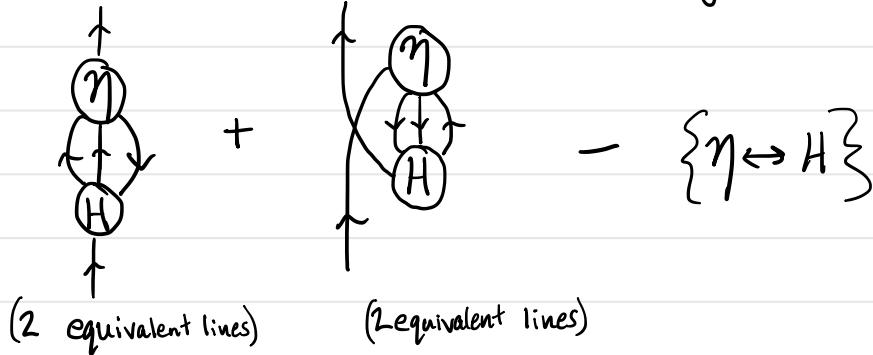
and we're calculating a particular contribution to  $C_{pq}$ .

Diagrammatically, the commutator term is

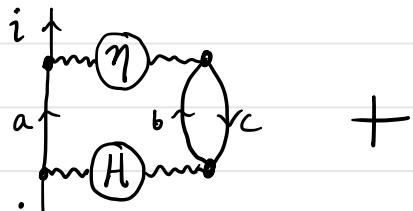
$$[\eta^{[2]}, H^{[2]}]^{[1]}$$



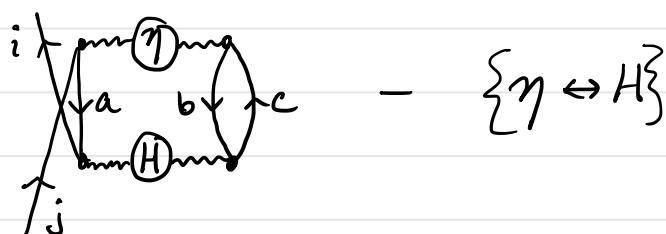
Note that the second diagram is the same as the first with  $\eta \leftrightarrow H$ , so let's focus on the first diagram. There are two ways to decorate this diagram with arrows, and we add both together



Next, we expand to Goldstone diagrams



$$l=1, h=1$$



$$l=1, h=2$$

$$\frac{1}{2}(-1)^{h+1} \eta_{icab} H_{abjc} \bar{n}_a \bar{n}_b n_c + \frac{1}{2}(-1)^{h+2} \eta_{abjc} H_{icab} n_a n_b \bar{n}_c - \{\eta \leftrightarrow H\}$$

So we obtain at last,

$$C_{ij} = \frac{1}{2} \sum_{abc} (\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) (\eta_{icab} H_{abjc} - H_{icab} \eta_{abjc}).$$

Note that this is just one term in the full commutator. The full flow equations, up to 2-body, are

$$\frac{d}{ds} E_0 = \sum_{ab} n_a \bar{n}_b (\eta_{ab} f_{ba} - f_{ab} \eta_{ba}) + \frac{1}{4} \sum_{abcd} n_a n_b \bar{n}_c \bar{n}_d (\eta_{abcd} \Gamma_{cdab} - \Gamma_{abdc} \eta_{cdab})$$

$$\begin{aligned} \frac{d}{ds} f_{ij} &= \sum_a (\eta_{ia} f_{aj} - f_{ia} \eta_{aj}) + \sum_{ab} (n_a \bar{n}_b - \bar{n}_a n_b) (\eta_{ab} \Gamma_{bij} - f_{ab} \eta_{bij}) \\ &\quad + \frac{1}{2} \sum_{abc} (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c) (\eta_{ciab} \Gamma_{abcj} - \Gamma_{ciab} \eta_{abcj}) \end{aligned}$$

$$\begin{aligned} \frac{d}{ds} \Gamma_{ijke} &= \sum_a \left[ (1-P_{ij})(\eta_{ia} \Gamma_{ajke} - f_{ia} \eta_{ajke}) - (1-P_{ke})(\eta_{ak} \Gamma_{ijae} - f_{ak} \eta_{ijae}) \right] \\ &\quad + \frac{1}{2} \sum_{ab} (\bar{n}_a \bar{n}_b - n_a n_b) (\eta_{ijab} \Gamma_{abke} - \Gamma_{ijab} \eta_{abke}) \\ &\quad + \sum_{ab} (n_a \bar{n}_b - \bar{n}_a n_b) (1-P_{ij})(1-P_{ke}) \eta_{aibk} \Gamma_{bjal}. \end{aligned}$$

Note that in the flow equations presented in eq (10.106) of LNP 936 some simplifications have been made, utilizing the hermiticity/antihemiticity of  $H$  and  $\eta$ . I have not done so here because for the Magnus formulation one needs a commutator of two antihemitian operators, and we can reuse this formula.

Diagrammatically,

$$\frac{d}{ds} E_0 = \text{Diagram } 1 + \text{Diagram } 2 + \{\text{rearrangements}\}$$

$$\frac{d}{ds} f_{pq} = \text{Diagram } 3 + \text{Diagram } 4 + \text{Diagram } 5 + \{\text{rearrangements}\}$$

$$\frac{d}{ds} \Gamma_{pqrs} = \text{Diagram } 6 + \text{Diagram } 7 + \text{Diagram } 8 + \{\text{rearrangements}\}$$

## Computational Scaling

Looking at the flow equations, we can see that the computational cost will scale as  $\Theta(N^6)$  where  $N$  is the number of single-particle states in our model space. To see this, look at the equation for  $\frac{d\Gamma}{dt} \Gamma_{ijkl}$ . This represents  $N^4$  equations because  $ijkl$  run from 0 to  $N$ . On the right hand side, we see summations over  $a, b$  which also run from 0 to  $N$ , so a naive implementation of the  $\Gamma$  flow equation would involve 6 nested loops, each running from 0 to  $N$ . Thus,  $N^6$  scaling, which is comparable with CCSD.

## Decoupling a ground state

Consider the action of the Hamiltonian on our reference state  $|\Phi\rangle$  (returning to the convention  $ijk \Rightarrow$  occupied,  $abc \Rightarrow$  unoccupied)

$$H|\Phi\rangle = E_0|\Phi\rangle + \sum_{ai} f_{ai} |\Phi_i^a\rangle + \frac{1}{4} \sum_{abij} \Gamma_{abij} |\phi_{ij}^{ab}\rangle$$

If we could make the second and third terms vanish by setting  $f_{ai}=0$ ,  $\Gamma_{abij}=0$  for all  $abij$ , then we'd have

$$H|\Phi\rangle = E_0|\Phi\rangle + 0$$

and  $|\Phi\rangle$  would be an eigenstate of  $H$  with energy  $E_0$ .

Our task is then to choose a generator  $\eta$  which suppresses  $f_{ai}$  and  $\Gamma_{abij}$ . One straightforward choice is the White generator (presented in a paper by Steven White):

$$\eta^{(\text{white})} = \sum_{ai} \frac{f_{ai}}{\Delta_{ai}} \{a_a^+ a_i\} + \frac{1}{4} \sum_{abij} \frac{\Gamma_{abij}}{\Delta_{abij}} \{a_a^+ a_b^+ a_j a_i\} - \text{h.c.}$$

The energy denominators  $\Delta_{ai}$ ,  $\Delta_{abij}$  can be chosen in various ways. The simplest choice is to use Moller-Plessett energy denominators:

$$\Delta_{ai}^{(\text{MP})} \equiv f_{aa} - f_{ii}, \quad \Delta_{abij}^{(\text{MP})} \equiv f_{aa} + f_{bb} - f_{ii} - f_{jj}.$$

We could also use Epstein-Nesbet energy denominators:

$$\Delta_{ai}^{(\text{EN})} = \langle \Phi_i^a | H | \Phi_i^a \rangle - \langle \Phi | H | \Phi \rangle$$

$$\Delta_{abij}^{(\text{EN})} = \langle \Phi_{ij}^{ab} | H | \Phi_{ij}^{ab} \rangle - \langle \Phi | H | \Phi \rangle.$$

In practice, the results are typically insensitive to this choice.

Looking at the White generator, we see that if  $f_{ai} = 0$  and  $\Gamma_{abij} = 0$ , then  $\eta = 0$ . So our desired form is a fixed point of the IMSRG flow.

With this generator, we flow to  $S \rightarrow \infty$  and the zero-body piece of the Hamiltonian  $E_0$  will become the ground state energy, up to errors due to the neglect of 3,4,... body operators.

There are other choices of generator which can lead to a decoupled ground state; however the White generator has nice numerical behavior when evolving to  $s \rightarrow \infty$ .

One small modification, also suggested by White, is to use an arctangent

$$\eta^W = \frac{1}{2} \sum_{a_i} \text{atan} \left( \frac{2f_{a_i}}{\Delta_{a_i}} \right) \{a_a^\dagger a_i\} + \frac{1}{8} \sum_{ab_{ij}} \text{atan} \left( \frac{2F_{ab_{ij}}}{\Delta_{ab_{ij}}} \right) \{a_a^\dagger a_b^\dagger a_j a_i\} - \text{h.c.}$$

The main advantage here is better handling of small energy denominators

### Implementation

Much of the model space and interaction book keeping code will be similar (or identical) to that used in MBPT or coupled cluster. The main new effort required for the IMSRG is 1) the implementation of the flow equations or, equivalently, of a commutator

$C = [A, B]$  where A and B are Fock space operators, and 2) the solution of the ordinary differential equation.

An Euler stepper method is sufficient as a first check, but you can do better with a more sophisticated adaptive ODE solver. Many such solvers are provided in freely available libraries such as Scipy, Boost, or SUNDIALS. You may also implement your own solver, e.g. Runge-Kutta.

As a separate point, we generally can't numerically integrate literally to  $s \rightarrow \infty$ . Instead, we should set some convergence criterion on e.g. the size of  $\eta$ , or the size of the MBPT 2 correction.

## IMSRG for nuclear matter

When treating nuclear matter, the flow equations are simplified due to the symmetries of the system, namely translational invariance, which implies momentum conservation. We also have angular momentum and isospin projection.

This means that  $f_{pq}$  is diagonal. The generators  $\eta$  and  $\Omega$  are also diagonal, but since they are antihermitian, they must be zero.

Also, the commutator of two diagonal matrices is zero, and so we can use simplified commutator expressions. Writing  $C = [A, B]$  we have

$$(0\text{-body}) \quad C_0 = \frac{1}{4} \sum_{abcd} n_a n_b \bar{n}_c \bar{n}_d (A_{abcd} B_{cdab} - B_{abcd} A_{cdab}) \quad *$$

$$(1\text{-body}) \quad C_{ij} = \frac{1}{2} \sum_{abc} (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c) (\eta_{ciab} \Gamma_{abcj} - \Gamma_{ciab} \eta_{abcj}) \quad *$$

$$\begin{aligned} (2\text{-body}) \quad C_{ijk\ell} = & - (B_{ii} + B_{jj} - B_{kk} - B_{ee}) A_{ijk\ell} \\ & + \frac{1}{2} \sum_{ab} (\bar{n}_a \bar{n}_b - n_a n_b) (A_{ijab} B_{abk\ell} - B_{ijab} A_{abk\ell}) \quad * \\ & + (1 - P_{ij})(1 - P_{k\ell}) \sum_{ab} (n_a \bar{n}_b - \bar{n}_a n_b) A_{aibk} B_{bjal}. \end{aligned}$$

Note that the terms marked with  $*$ 's are suggestive of a matrix-matrix multiplication.

## Particle-hole transformation

If you implement the above expressions in a straightforward way, the last term will likely be painfully slow for all but the smallest model spaces. This is due to the need to look matrix elements up based on orbit index in an inefficient way.

Things can be greatly improved by using what is called a particle-hole transformation. Essentially, we just shift the ordering of the creation/annihilation operators to make things more convenient.

Our two body operator is written in normal ordered form as

$$A = \frac{1}{4} \sum_{pqrs} A_{pqrs} \{ a_p^+ a_q^+ a_s a_r \}.$$

Now the trick: interpret the annihilation of a particle as the creation of a hole:  $a_s \equiv h_s^+$ .

Likewise  $a_q^+ \equiv h_q$  so

$$A = \frac{1}{4} \sum_{pqrs} A_{pqrs} \{ a_p^+ h_q h_s^+ a_r \}$$

$$= -\frac{1}{4} \sum_{pqrs} A_{pqrs} \{ a_p^+ h_s^+ h_q a_r \}$$

Now we define the coefficient in front of the  $\{ \}$  such that

$$A = \frac{1}{4} \sum_{pqrs} \bar{A}_{pqrs} \{ a_p^+ h_s^+ h_q a_r \}.$$

Evidently,

$$\bar{A}_{p\bar{s}r\bar{q}} = -A_{pqrs}.$$

In terms of these particle-hole matrix elements, the last term in the commutator expression can be rearranged to be

$$\bar{C}_{i\bar{p}k\bar{j}} = (1-P_{ij})(1-P_{ke}) \sum_{ab} (n_a \bar{n}_b - \bar{n}_a n_b) \bar{A}_{i\bar{z}a\bar{b}} \bar{B}_{a\bar{b}k\bar{j}}.$$

This has the structure of a matrix-matrix multiplication, and in practice this is much faster than the straightforward sum over indices.

In the end, we're interested in  $C_{ijke}$ , not  $\bar{C}_{i\bar{p}k\bar{j}}$ , so we need to transform back. The workflow should look something like:

- 1) Transform A & B to the ph representation.
- 2) Perform the matrix-matrix multiplication (don't forget the  $n_a \bar{n}_b - \bar{n}_a n_b$  factor).
- 3) Transform back to the particle-particle representation.
- 4) Do the antisymmetrizations  $(1-P_{ij})(1-P_{ke})$ .

To summarize, this ph transformation just amounts to temporarily switching the order of the creation/annihilation operators. After the matrix multiplication, we switch back.

## Solving the flow equations

A simple implementation would proceed along the following lines

1) Obtain the normal ordered Hamiltonian  $H(0)$

Inside a for/while/do loop

2) Calculate the generator  $\eta(H(s))$

3) Evaluate the commutator  $[\eta(s), H(s)]$

4) Choose a step size  $ds$

5) Update  $H(s+ds) = ds \cdot [\eta(s), H(s)]$

6) Check for convergence by evaluating, e.g. MBPT2 on  $H(s)$ , or  $\frac{dE_0}{ds}$ .

One can also implement more sophisticated solvers, e.g. a 4th order Runge-Kutta:

$$dH^{[1]} = [\eta, H]$$

$$dH^{[2]} = [\eta(H + \frac{ds}{2} dH^{[1]}), H + \frac{ds}{2} dH^{[1]}]$$

$$dH^{[3]} = [\eta(H + \frac{ds}{2} dH^{[2]}), H + \frac{ds}{2} dH^{[2]}]$$

$$dH^{[4]} = [\eta(H + ds dH^{[3]}), H + ds dH^{[3]}]$$

$$H(s+ds) = \frac{ds}{6} (dH^{[1]} + 2dH^{[2]} + 2dH^{[3]} + dH^{[4]})$$

Note that this requires 4 commutator evaluations per step, but it's worth it since our error is proportional to  $ds^5$  while the Euler stepper has an error proportional to  $ds^2$ . So Runge-Kutta with  $ds=0.1$  has comparable accuracy to the Euler method with  $ds \approx 0.003$ .

## The Magnus formulation of IMSRG

There is another formulation of the IMSRG which has several advantages - both numerical and formal - over direct integration of the flow equations.

Recall that our starting point for SRG was a unitary transformation

$$H(s) = U(s) H(0) U^\dagger(s).$$

Any unitary transformation may be expressed as the exponential of some antihermitian operator, which we denote  $\Omega$ , said to be the generator of the transformation

$$U(s) = e^{\Omega(s)}$$

$\Omega$  is antihermitian so  $\Omega^\dagger = -\Omega \Rightarrow U^\dagger U = e^{-\Omega} e^\Omega = \mathbb{1}$ .

Given  $\Omega$ , we can evaluate the transformed Hamiltonian using the series expansion of the exponential

$$\begin{aligned} H(s) &= e^{\Omega(s)} H(0) e^{-\Omega(s)} \\ &= H(0) + [\Omega(s), H(0)] + \frac{1}{2} [\Omega(s), [\Omega(s), H(0)]] + \frac{1}{3!} [\Omega(s), [\Omega(s), [\Omega(s), H(0)]]] + \dots \end{aligned}$$

This series is formally infinite. However, the (suitably defined) norm of a commutator is bounded:

$$\|[H, \Omega]\| \leq 2 \|\Omega\| \cdot \|H\|.$$

The next nested commutator is then  $\|[H, [\Omega, H]]\| \leq 4 \|\Omega\|^2 \|H\|$ .

The  $n$ th nested commutator is bounded by

$$\left\| \underbrace{[\mathcal{L}, [\dots [\mathcal{L}, H]]_-.]}_{n \text{ commutators}} \right\| \leq (2\|\mathcal{L}\|)^n \|H\|.$$

We can easily see that if  $2\|\mathcal{L}\| < 1$ , the series will converge. An application of Taylor's theorem reveals that for any finite convergence requirement, only a finite number of terms are needed. In reality, the magnitude of the commutator is smaller than its upper bound, and the series converges even if  $2\|\mathcal{L}\| > 1$ . Moreover, in most calculations the series converges within 5-10 nested commutators.

Note the connection to Coupled Cluster, where the nested commutator expression formally terminates, at the cost of Hermiticity. Here, we maintain a Hermitian Hamiltonian, but our series does not formally terminate and we must rely on numerical convergence.

So, how can we obtain  $\mathcal{L}$ ? Imagine we have found  $\mathcal{L}(s)$ , and we wish to find  $\mathcal{L}(s+\delta s)$ . Working backwards from our expansion of the exponential form, we see

$$H(s+\delta s) = H(s) + \delta s [\eta, H(s)] + \mathcal{O}(\delta s^2)$$

implies

$$\begin{aligned} H(s+\delta s) &= e^{\eta \delta s} H(s) e^{-\eta \delta s} \\ &= e^{\eta \delta s} e^{\mathcal{L}(s)} H(0) e^{-\mathcal{L}(s)} e^{-\eta \delta s} \\ &= e^{\mathcal{L}(s+\delta s)} H(0) e^{-\mathcal{L}(s+\delta s)} \end{aligned}$$

So we see that

$$e^{\Omega(s+\delta s)} = e^{\Omega(s)} e^{\eta(s) \delta s}.$$

Now if  $\Omega$  and  $\eta$  were just numbers, we would immediately have  $\Omega(s+\delta s) = \Omega(s) + \eta(s) \delta s$ . However, these are in general non commuting operators and so

$$e^{\Omega(s)} e^{\eta(s) \delta s} \neq e^{\Omega(s) + \eta(s) \delta s}.$$

To combine the two exponentials into one, we need to use the Baker-Campbell-Hausdorff formula

$$\log(e^A e^B) = A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] + [B, [B, A]]) + \dots$$

Or, plugging in our operators

$$\Omega(s+\delta s) = \Omega(s) + \eta(s) \delta s + \frac{1}{2} [\Omega(s), \eta(s)] \delta s + \frac{1}{12} \left( [\Omega(s), [\Omega(s), \eta(s)]] \delta s + [\eta(s), [\eta(s), \Omega(s)]] \delta s^2 \right) + \dots$$

Taking  $\delta s$  infinitesimal, we can keep only linear terms  $\delta s$  and obtain a flow equation for  $\Omega(s)$

$$\frac{d}{ds} \Omega(s) = \eta(s) + \frac{1}{2} [\Omega(s), \eta(s)] + \frac{1}{12} [\Omega(s), [\Omega(s), \eta(s)]] + \dots$$

Writing the  $k$ th nested commutator as  $\text{ad}_{\Omega}^k(\eta)$ , this may be expressed as

$$\frac{d}{ds} \Omega(s) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}_{\Omega}^k(\eta)$$

where  $B_k$  is the  $k$ th Bernoulli number.

We have encountered a second infinite series of nested commutators. While as before there is no formal truncation, the series converges quickly in most applications.

In fact, being a little sloppy in evaluating  $\frac{d\Omega}{ds}$  is not as serious as being sloppy with  $\frac{dH}{ds}$ . Even if we truncate the series prematurely,  $\Omega$  will be antihermitian and so  $e^{\Omega}$  will be a unitary transformation.

Of course, because we truncate the transformation of  $H$  to 2-body operators, the transformation is not truly unitary. Nevertheless, the flow equation for  $\Omega$  is much more forgiving of simple integrators than the flow for  $H$  is; a simple Euler stepper will do.

A second advantage of the Magnus approach is that once we've obtained  $\Omega(s)$  that achieves our desired decoupling, we may transform another operator corresponding to some observable (e.g. the radius) by

$$\begin{aligned}\mathcal{O}(s) &= e^{\Omega(s)} \mathcal{O}(0) e^{-\Omega(s)} \\ &= \mathcal{O}(0) + [\Omega(s), \mathcal{O}(0)] + \frac{1}{2} [\Omega(s), [\Omega(s), \mathcal{O}(0)]] + \dots\end{aligned}$$

We may even write  $\Omega$  to disk and come back months later to transform some observable we decided is interesting.

In contrast, when flowing  $H$  (the "standard" way) we need to carry along any operators as we flow, evaluating

$$\frac{d}{ds} \mathcal{O}(s) = [\eta(s), \mathcal{O}(s)]$$

which ends up requiring many more commutator evaluations.

The gain is especially significant for the transformation of operators which carry angular momentum, e.g. the electric quadrupole operator, because commutators are significantly more expensive for these operators.

The Magnus formulation also facilitates perturbative corrections to our neglect of higher body operators. For example, for a 2-body  $H$  and a 2-body  $\Omega$ , the leading correction to the energy  $E_0$  comes at 3 nested commutators

$$\delta E_0 = \frac{1}{3!} [\Omega_2, [\Omega_2, [\Omega_2, H_3]_3]_{1,2}]_0 + \mathcal{O}(s^4)$$

Here the subscripts indicate terms of a given particle rank. Of course, our transformation induces a 3-body interaction  $W(s)$  and so our reference is not truly decoupled. We may either evaluate the effect of  $W$  in perturbation theory, or approximate the 3-body piece of  $\Omega_2$  as  $\Omega_2^{(3)} = \frac{W_{abcijk}}{\Delta_{abcijk}}$  and evaluate  $\delta E = [\Omega_2^{(3)}, W]_0$ , the result is the same, and can be evaluated with  $n^7$  scaling. Importantly, this is just one  $n^7$  evaluation at the end. The flow is still performed at  $n^6$  scaling. We will not delve further into this - the point is that the Magnus formulation makes perturbative approximations of IMSRG(3) more transparent and easier to implement.

## Connections to Coupled Cluster theory

Using the Magnus formulation, we may highlight some similarities to coupled cluster.

The ground state energy is given by

$$\begin{aligned}
 E_{\text{IMSRG}} &= (e^{\Omega} H e^{-\Omega})_{ab} \\
 &= E_0 + [\Omega, H]_{ab} + \frac{1}{2} [\Omega, [\Omega, H]]_{ab} + \dots \\
 &= E_0 + \sum_{ia} (\Omega_{ia} f_{ai} - f_{ia} \Omega_{ai}) + \frac{1}{4} \sum_{abij} (\Omega_{ijab} \Gamma_{abij} - \Gamma_{abij} \Omega_{ijab}) \\
 &\quad + \dots
 \end{aligned}$$

The Coupled cluster singles+doubles energy is

$$E_{\text{CCSD}} = E_0 + \sum_{ia} t_i^a f_{ia} + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} \Gamma_{ijab}$$

The decoupling conditions for the IMRG fixed point are

$$\langle \phi_i^a | e^{\Omega} H e^{-\Omega} | \phi \rangle = 0$$

$$\langle \phi_{ij}^{ab} | e^{\Omega} H e^{-\Omega} | \phi \rangle = 0$$

Evaluating the commutator for the second condition under the assumption  $\Omega_{ia} \approx 0$ ,  $f_{pq} = \epsilon_p \delta_{pq}$  we have

$$0 = \Gamma_{abij} + (\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b) \Omega_{abij}$$

$$+ \frac{1}{2} \sum_{cd} (\Omega_{abcd} \Gamma_{cdij} - \Gamma_{abcd} \Omega_{cdij}) - \frac{1}{2} \sum_{ke} (\Omega_{abke} \Gamma_{keij} - \Gamma_{abke} \Omega_{keij})$$

$$+ P(ij|ab) \sum_{ck} (\Omega_{kaci} \Gamma_{cbkj} - \Gamma_{kaci} \Omega_{cbkj})$$

$$+ \mathcal{O}(\omega^2)$$

Comparing this to the CCD amplitude equation, we have

$$0 = \Gamma_{abij} + (\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j) t_{ij}^{ab}$$

$$+ \frac{1}{2} \sum_{cd} \Gamma_{abcd} t_{ij}^{cd} + \frac{1}{2} \sum_{ke} \Gamma_{keij} t_{ke}^{ab}$$

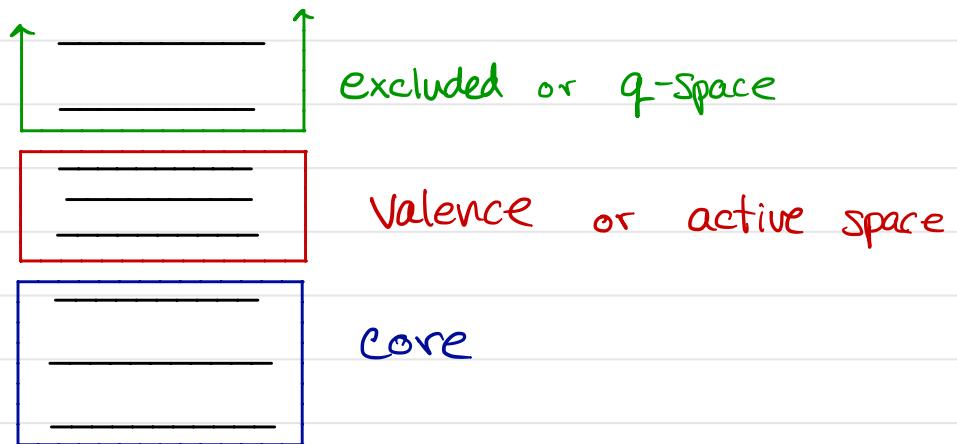
$$+ P(ij|ab) \sum_{kc} \Gamma_{kbcj} t_{ik}^{ac} + \mathcal{O}(t^2)$$

From this it should be clear that the two approaches are doing similar things. In fact, the methods have equivalent content through 3rd order in MBPT, and there is one class of 4th order diagram which is undercounted in IMSRG(2) by a factor  $\frac{1}{2}$ . One can play some games to restore the proper counting of this diagram without affecting the scaling of the method.

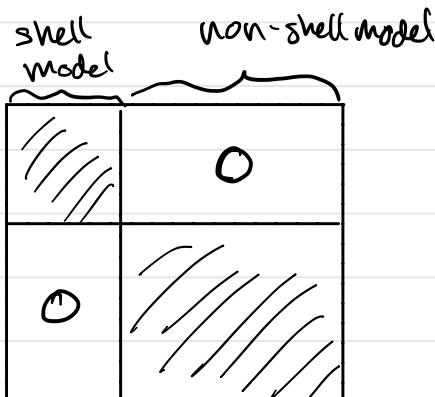
## Extensions

### Valence Space /MSRG

One straightforward extension of our discussion of the IMRG is to decouple a valence space rather than a single reference configuration. The basic idea is that rather than splitting our single particle states into occupied/unoccupied, we use 3 designations - core, valence, and excluded



We designate configurations with all core orbits occupied and all excluded orbits unoccupied as "shell model" configurations. Our aim is to use the IMRG to block-diagonalize the Hamiltonian, decoupling the shell model configurations from all other configurations.



Then we diagonalize exactly in the smaller shell model subspace.

To achieve this, we must adjust our definition of which terms in the Hamiltonian are off-diagonal. These should be terms that can connect a shell model configuration to a non-shell model configuration, namely,

$$H^{od} = \{ f_{pc} + \underline{f_{qv}} + \underline{\Gamma_{ppcc}} + \underline{\Gamma_{ppvc}} + \underline{\Gamma_{qpvv}} \}$$

I've used  $p = \{ v, q \}$  to make things more compact. The terms which do not arise for the single-reference decoupling are underlined in red.

Our generator  $\eta$  should be chosen to suppress these terms.

In practice it turns out to be advantageous to perform this decoupling in two steps. First we decouple the core, then we decouple the valence space.

## Equations of Motion IMSRG

Another straightforward extension is to use an IMSRG-decoupled ground state as the starting point for a truncated CI expansion.

We can express an excited state  $|4_v\rangle$  as an excitation operator  $\chi_v$  acting on the IMSRG ground state.

$$|4_v\rangle = \chi_v |4_{gs}\rangle$$

The Schrödinger equation then tells us

$$H \chi_v |4_{gs}\rangle = E_v \chi_v |4_{gs}\rangle$$

also,

$$\chi_v H |4_{gs}\rangle = E_0 \chi_v |4_{gs}\rangle$$

$$\text{so } [H, \chi_v] |4_{gs}\rangle = (E_v - E_0) \chi_v |4_{gs}\rangle.$$

This equation can be solved for the unknowns  $E_v, \chi_v$  by the Lanczos algorithm, with a commutator evaluation in place of a matrix-vector multiplication.

The form of the operator  $\chi_v$  is

$$\chi_v = \sum_{ai} \chi_v^{ai} \{a_a^\dagger a_i\} + \frac{1}{4} \sum_{abij} \chi_v^{abij} \{a_a^\dagger a_b^\dagger a_j a_i\} + \dots$$

Since we're truncating our commutators at the

2-body level, our excited states will be linear combinations of  $1p1h$  and  $2p2h$  excitations. This is evidently equivalent to CI with singles and doubles, or CISD. The only difference from the earlier discussion by Morten is that we use the transformed Hamiltonian and so implicitly we are using the correlated ground state rather than e.g. Hartree-Fock.

## Multireference IMRG

A third extension can be made by using a more complicated reference which already has some correlations built in. This is useful for open shell nuclei where a single Slater determinant may not be a sufficient zero order approximation of the ground state, so that  $|\phi\rangle \neq |f\rangle$  and the normal ordering approximation becomes inefficient.

In order to use a correlated reference, we need to generalize Wick's theorem. We still define normal order to be an ordering which vanishes in the reference, i.e.

$$\langle \phi | \{\alpha_1, \alpha_2, \dots, \alpha_n\} | \phi \rangle = 0.$$

However, because our reference is correlated, it cannot be characterized simply by occupation numbers, and we will need to introduce the notion of irreducible n-body density matrices.