Relevant IMSRG equations

Normal-ordered operators:

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

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

$$\Gamma_{pqrs} = V_{pqrs} + \sum_i n_i V^{(3)}_{pqirsi} \tag{3}$$

$$W_{pqrstu} = V^{(3)}_{pqrstu} \tag{4}$$

IMSRG flow equations. Note that here we do not follow the CC/MBPT convetion that ijk are hole indices and abc are particle indices. Instead, abc are used for interal (contracted) indices which are summed over, and ijk are external indices.

$$\frac{d}{ds}E_0 = \sum_{ab} n_a \bar{n}_b \left(\eta_{ab} f_{ba} - f_{ab}\eta_{ba}\right) + \frac{1}{4}\sum_{abcd} n_a n_b \bar{n}_c \bar{n}_d \left(\eta_{abcd}\Gamma_{cdab} - \Gamma_{abcd}\eta_{cdab}\right) \tag{5}$$

$$\begin{aligned}\frac{d}{ds}f_{ij} = \sum_a \left(\eta_{ia} f_{aj} - f_{ia}\eta_{aj}\right) + \sum_{ab}(n_a\bar{n}_b - \bar{n}_a n_b)\left(\eta_{ab}\Gamma_{biaj} - f_{ab}\eta_{biaj}\right) \\ + \frac{1}{2}\sum_{abc}(n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c)\left(\eta_{ciab}\Gamma_{abcj} - \Gamma_{ciab}\eta_{abcj}\right)\end{aligned} \tag{6}$$

$$\begin{aligned}\frac{d}{ds}\Gamma_{ijkl} = &\sum_a \left[(1 - P_{ij}\left(\eta_{ia}\Gamma_{ajkl} - f_{ia}\eta_{ajkl}\right) - (1 - P_{kl})\left(\eta_{ak}\Gamma_{kjal} - f_{ak}\eta_{ijal}\right)\right] \\ &+ \frac{1}{2}\sum_{ab}(\bar{n}_a\bar{n}_b - n_a n_b)\left(\eta_{ijab}\Gamma_{abkl} - \Gamma_{ijab}\eta_{abkl}\right) \\ &+ (1 - P_{ij})(1 - P_{kl})\sum_{ab}(n_a\bar{n}_b - \bar{n}_a n_b)\eta_{aibk}\Gamma_{bjal}\end{aligned} \tag{7}$$

The White generator:

$$\eta^{\mathrm{Wh}}_{ai} = \frac{f_{ai}}{\Delta_{ai}} - h.c. \tag{8}$$

$$\eta^{\mathrm{Wh}}_{abij} = \frac{\Gamma_{abij}}{\Delta_{abij}} - h.c. \tag{9}$$

Here we use the Moller-Plesset energy denominators. Other choices are possible, but these will suffice for our purposes.

$$\Delta_{ai} = f_{aa} - f_{ii} \tag{10}$$

$$\Delta_{abij} = f_{aa} + f_{bb} - f_{ii} - f_{jj} \tag{11}$$

For nuclear matter, momentum conservation restricts one-body operators to be diagonal. This allows for some simplification of flow equations:

$$\frac{d}{ds}E_0 = \frac{1}{4}\sum_{abcd} n_a n_b \bar{n}_c \bar{n}_d \left(\eta_{abcd}\Gamma_{cdab} - \Gamma_{abcd}\eta_{cdab}\right) \tag{12}$$

$$\frac{d}{ds}f_{ij} = \frac{1}{2}\sum_{abc}(n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c)\left(\eta_{ciab}\Gamma_{abcj} - \Gamma_{ciab}\eta_{abcj}\right) \tag{13}$$

$$\begin{aligned}\frac{d}{ds}\Gamma_{ijkl} &= (A_{ii} + A_{jj} - A_{kk} - A_{ll})B_{ijkl} - (B_{ii} + B_{jj} - B_{kk} - B_{ll})A_{ijkl} \\ &+ \frac{1}{2}\sum_{ab}(\bar{n}_a\bar{n}_b - n_a n_b)\left(\eta_{ijab}\Gamma_{abkl} - \Gamma_{ijab}\eta_{abkl}\right) \\ &+ (1 - P_{ij})(1 - P_{kl})\sum_{ab}(n_a\bar{n}_b - \bar{n}_a n_b)\eta_{aibk}\Gamma_{bjal}\end{aligned} \tag{14}$$

Benchmarking the pairing model

Pairing model with 4 particles, in 4 doubly degenerate levels, for $\delta = 1$ and $g = +0.5$

Solving the IMSRG flow equation with a simple Euler step method with step size $ds = 0.1$. E_0 is the zero-body piece of the flowing Hamiltonian $H(s)$. EMBPT2 is the second order MBPT energy using $H(s)$, and dE/ds is the zero body part of $[\eta(s), H(s)]$.

s	E_0	EMBPT2	dE/ds
0.0	1.50000	-0.0623932	0.0000000
0.1	1.48752	-0.0531358	-0.1247860
0.2	1.47689	-0.0453987	-0.1062720
0.3	1.46781	-0.0388940	-0.0907975
0.4	1.46004	-0.0333983	-0.0777880
0.5	1.45336	-0.0287359	-0.0667967

The same numbers as before, but now the $[\eta_{2b}, H_{2b}]_{2b}$ particle-hole commutator term is omitted.

s	E_0	EMBPT2	dE/ds
0	1.5	-0.0623932	0
0.1	1.48752	-0.0531358	-0.124786
0.2	1.47689	-0.0453551	-0.106272
0.3	1.46782	-0.0387878	-0.0907102
0.4	1.46007	-0.0332251	-0.0775756
0.5	1.45342	-0.0284994	-0.0664503
0.6	1.44772	-0.0244746	-0.0569988
0.7	1.44283	-0.0210395	-0.0489492