

In-medium SRG to the nuclear shell model

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Abstract

In-medium SRG equations for nuclear matter and finite system have been derived in M-scheme and jj-coupled formalism. Some choices of generators have been tested and the convergence has been checked. TBME'S for the nuclear shell model are shown.

I. BASICS OF SRG

Consider a Hamiltonian that we split into diagonal and off-diagonal parts

$$H = H_d + H_{od} \quad (1)$$

This could be a simple 1-body Hamiltonian, or it could be a complicate nuclear Hamiltonian with 2- and 3-body forces acting in a many-body Hilbert space. Suppose that we want to construct a unitarily equivalent Hamiltonian where the dominant piece has an operator structure given by H_d . The SRG provides a prescription to construct the appropriate unitary transformation. Formally write the transformed Hamiltonian as

$$H(s) = U^\dagger(s) H U(s) \equiv H_d(s) + H_{od}(s), \quad (2)$$

where s is a continuous parameter and $U(0) = 1, H(0) = H$. Taking d/ds on both sides then gives

$$\frac{dH(s)}{ds} = [\eta(s), H(s)], \quad (3)$$

where the anti-hermitian generator of the transformation is given by

$$\eta(s) = \frac{dU^\dagger}{ds} U = -\eta^\dagger(s). \quad (4)$$

We can formally write the unitary transformation as an s -ordered exponential,

$$U(s) = \mathcal{S} \exp \left(- \int_0^s ds' \eta(s') \right). \quad (5)$$

Wegner's idea was to take the following ansatz for the generator to drive the Hamiltonian towards the diagonal in the eigenbasis of H_d (i.e., $H_d|i\rangle = \epsilon_i|i\rangle$),

$$\eta = [H_d, H] = [H_d, H_{od}]. \quad (6)$$

From the definition of η one can show

$$\frac{d}{ds} \text{Tr} (H_{od}^2) = 2\text{Tr}(\eta^2) = -2\text{Tr}(\eta^\dagger \eta) \leq 0 \quad (\eta \text{ is positive semi-definite}), \quad (7)$$

which demonstrates that the strength of H_{od} decay with increasing s . The following conditions are sufficient for Wegner's choice of generator to work properly:

$$\text{Tr} (H_d H_{od}) = 0, \quad (8)$$

$$\text{Tr} \left(\frac{dH_d}{ds} H_{od} \right) = 0, \quad (9)$$

where the trace is taken over the whole many-body Hilbert space.

II. FREE SPACE SRG

$$\frac{d}{ds}V_s(k, k') = -(k^2 - k'^2)^2 V_s(k, k') + \frac{2}{\pi} \int_0^\infty dq q^2 (k^2 + k'^2 - 2q^2) V_s(k, q) V_s(q, k'). \quad (10)$$

III. IN-MEDIUM SRG

The Hamiltonian is given as

$$\hat{H} = \sum_{ij} T_{ij} i^\dagger j + \frac{1}{2!^2} \sum_{ijkl} \{ij|V_2|kl\} i^\dagger j^\dagger lk + \frac{1}{3!^2} \sum_{ijklmn} \{ijk|V_3|lmn\} i^\dagger j^\dagger k^\dagger nml + \dots \quad (11)$$

With the aid of Wick's theorem, we can rewrite \hat{H} as

$$\hat{H} = E_0 + \sum_{kk'} g_{kk'} N(k^\dagger k') + \frac{1}{2!^2} \sum_{kpqr} \Gamma_{kpqr} N(k^\dagger p^\dagger r q) + \frac{1}{3!^2} \sum_{kpqrst} \{kpq|V_3|rst\} N(k^\dagger p^\dagger q^\dagger t sr), \quad (12)$$

where E_0, f_k, Γ_{pqrs} are given by

$$E_0 = \langle H \rangle_0 = \sum_k T_{kk} n_k + \frac{1}{2} \sum_{ij} \{ij|V_2|ij\} n_i n_j + \frac{1}{6} \sum_{ijk} \{ijk|V_3|ijk\} n_i n_j n_k \quad (13)$$

$$g_{ij} = T_{ij} + \sum_k \{ik|V_2|jk\} n_k + \frac{1}{2} \sum_{kl} \{ikl|V_3|jkl\} n_k n_l \quad (14)$$

$$\{kp|\Gamma|qr\} = \{kp|V_2|qr\} + \frac{1}{4} \sum_i \{kpi|V_3|qri\} n_i \quad (15)$$

In an infinite homogeneous system, from momentum conservation, one can show that the operator \hat{g} is always diagonal.

$$g_{ij} = \delta_{ij} f_i, \quad (16)$$

$$\text{where } f_i = \epsilon_i + \sum_k \{ik|V_2|ik\} n_k + \frac{1}{2} \sum_{kl} \{ikl|V_3|ikl\} n_k n_l \quad (17)$$

In following discussion, we truncate the Hamiltonian (and generator $\hat{\eta}$) to normal-ordered two-body operators. The Hamiltonian is divided into two parts,

$$\hat{H} = \overline{\langle H \rangle + \hat{g}^d + \hat{\Gamma}^d} + \overline{\hat{g}^{od} + \hat{\Gamma}^{od}} \quad (18)$$

$$= \hat{H}^d + \hat{H}^{od} \quad (19)$$

where,

$$\hat{g} = \hat{g}^d + \hat{g}^{od} = \sum_{12} N(1^\dagger 2)(g_{12}^d + g_{12}^{od}) \quad (20)$$

$$\hat{\Gamma} = \hat{\Gamma}^d + \hat{\Gamma}^{od} = \sum_{1234} N(1^\dagger 2^\dagger 43)(\Gamma_{1234}^d + \Gamma_{1234}^{od}). \quad (21)$$

$$\Gamma_{1234}^d = 0 \quad (\epsilon_1 + \epsilon_2 \neq \epsilon_3 + \epsilon_4), \quad \Gamma_{1234}^{od} = 0 \quad (\epsilon_1 + \epsilon_2 = \epsilon_3 + \epsilon_4), \quad (22)$$

$$g_{12}^d = 0 \quad (\epsilon_1 \neq \epsilon_2), \quad g_{12}^{od} = 0 \quad (\epsilon_1 = \epsilon_2). \quad (23)$$

The generator is written as

$$\hat{\eta} = [\hat{H}^d, \hat{H}^{od}] = [\hat{g}^d + \hat{\Gamma}^d, \hat{g}^{od} + \hat{\Gamma}^{od}] \quad (24)$$

IV. FUNDAMENTAL COMMUTATORS

It is convenient to first calculate all the commutators which we need. We write one- and two-body operators as

$$\hat{A}^{1b} = \sum_{12} A_{12}^{1b} 1^\dagger 2, \quad \hat{A}^{2b} = \frac{1}{4} \sum_{1234} A_{1234}^{2b} 1^\dagger 2^\dagger 43, \quad (25)$$

assuming that the two-body matrix elements (TBME's) are antisymmerized,

$$A_{1234} = -A_{2134} = -A_{1243} = A_{2143} \quad (26)$$

The important commutators are obtained as follows.

$$[\hat{A}^{1b}, \hat{B}^{2b}]_{2b} = \frac{1}{4} \sum_{1234} \sum_a N(1^\dagger 2^\dagger 43) \{A_{1a}B_{a234} + A_{2a}B_{1a34} - A_{a3}B_{12a4} - A_{a4}B_{123a}\} \quad (27a)$$

$$[\hat{A}^{1b}, \hat{B}^{2b}]_{1b} = \sum_{12} N(1^\dagger 2) \left\{ \sum_{ab} (n_a - n_b) A_{ab} B_{b1a2} \right\} \quad (27b)$$

$$[\hat{A}^{1b}, \hat{B}^{1b}]_{1b} = \sum_{12} N(1^\dagger 2) \left\{ \sum_a (A_{1a}B_{a2} - B_{1a}A_{a2}) \right\} \quad (27c)$$

$$[\hat{A}^{1b}, \hat{B}^{1b}]_{0b} = \sum_{12} A_{12} B_{21} (n_1 - n_2) \quad (27d)$$

$$[\hat{A}^{2b}, \hat{B}^{2b}]_{2b} = \frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \left\{ \frac{1}{2} \sum_{ab} (A_{12ab}B_{ab34} - B_{12ab}A_{ab34})(1 - n_a - n_b) \right. \\ \left. + \sum_{ab} (n_a - n_b)(A_{a1b3}B_{b2a4} - A_{a2b3}B_{b1a4} - A_{a1b4}B_{b2a3} - A_{a2b4}B_{b1a3}) \right\} \quad (27e)$$

$$[\hat{A}^{2b}, \hat{B}^{2b}]_{1b} = \sum_{12} N(1^\dagger 2) \left\{ \frac{1}{2} \sum_{abc} (A_{c1ab}B_{abc2} - B_{c1ab}A_{abc2})(\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) \right\} \quad (27f)$$

$$[\hat{A}^{2b}, \hat{B}^{2b}]_{0b} = \frac{1}{4} \sum_{1234} (A_{1234}B_{3412} - B_{1234}A_{3412}) n_1 n_2 \bar{n}_3 \bar{n}_4 \quad (27g)$$

V. NUCLEAR MATTER

We apply the plane wave s.p. basis. The \hat{g} is diagonal in this basis. If one follows the definition of Wegner's choice, the generator is,

$$\hat{\eta}^{NM} = [\hat{g} + \hat{\Gamma}^d, \hat{\Gamma}^{od}]. \quad (28)$$

We approximate this as

$$\hat{\eta}^{NM} = [\hat{g}, \hat{\Gamma}], \quad (29)$$

assuming that the difference between these two generators is negligible. In this case, the generator of Eq. (29) is written as

$$\hat{\eta}^{NM}(s) = [\hat{g}(s), \hat{\Gamma}(s)] = \frac{1}{4} \sum_{ab1234} g_{ab}(s) \Gamma_{1234} [N(a^\dagger b), N1^\dagger 2^\dagger 43]. \quad (30)$$

$$= \frac{1}{4} \sum_{1234} (f_1 + f_2 - f_3 - f_4) \Gamma_{1234} N(1^\dagger 2^\dagger 43) \equiv \frac{1}{4} \sum_{1234} \eta_{1234}^{NM} N(1^\dagger 2^\dagger 43), \quad (31)$$

where

$$\eta_{1234}^{NM} \equiv (f_{12} - f_{34}) \Gamma_{1234}, \quad f_{ij} \equiv f_i + f_j. \quad (32)$$

This generator satisfies the symmetry relations bellow

$$\eta_{1234}^{NM} = -\eta_{3412}^{NM} \text{ (antihermitian)} \quad (33)$$

$$\eta_{1234}^{NM} = -\eta_{2134}^{NM} = \eta_{2143}^{NM} = -\eta_{1243}^{NM} \text{ (antisymmetry)} \quad (34)$$

It is clear that we find normal-ordered zero-, one-, and two-body (and truncated higher-body) terms in the evaluation of the flow equation. Finally one obtains

$$\frac{dE_0}{ds} = \frac{1}{2} \sum_{1234} (f_{12} - f_{34}) |\Gamma_{1234}|^2 n_1 n_2 \bar{n}_3 \bar{n}_4 \quad (35)$$

$$\frac{df_1}{ds} = \sum_{abc} (f_{c1} - f_{ab}) |\Gamma_{1cab}|^2 (\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) \quad (36)$$

$$\begin{aligned} \frac{d\Gamma_{1234}}{ds} = & -(f_{12} - f_{34})^2 \Gamma_{1234} + \frac{1}{2} \sum_{ab} (f_{12} + f_{34} - 2f_{ab}) \Gamma_{12ab} \Gamma_{ab34} (1 - n_a - n_b) \\ & + \sum_{ab} (n_a - n_b) [f_{a1} - f_{b3} - f_{b2} + f_{a4}) \Gamma_{a1b3} \Gamma_{b2a4} - (f_{a2} - f_{b3} - f_{b1} + f_{a4}) \Gamma_{a2b3} \Gamma_{b1a4}] \end{aligned} \quad (37)$$

VI. A SIMPLE MODEL

Let us consider a simple model to illustrate the feature of (Im-medium) SRG. We take three-level model as an example. The Hailtonian is

$$H = \sum_{i=1}^3 \epsilon_i a_i^\dagger a_i + \sum_{i \neq j} V_{ij} a_i^\dagger a_j \quad (38)$$

We assume that only $V_{12} = V_{21}$ do not vanish. The eigenvalues for the one-particle system (spand by $|1\rangle, |2\rangle, |3\rangle$) are

$$E_{1,2}^{1p} = \frac{\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4V_{12}^2}}{2}, \quad E_3 = \epsilon_3 \quad (39)$$

And the eigenvalues for the two-particle system (spand by $|12\rangle, |13\rangle|23\rangle$) are

$$E_1^{2p} = \epsilon_1 + \epsilon_2, E_{2,3} = \epsilon_3 + \frac{\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4V_{12}^2}}{2}. \quad (40)$$

The eigenvalue for three particle system, which is just 1-dim, is $E^{3p} = \epsilon_1 + \epsilon_2 + \epsilon_3$. Now the level $|1\rangle$ is under the Femi sea. The Hamiltonian is rewritten taking the normal-ordering,

$$H = \epsilon_1 + \sum_{i=1}^3 \epsilon_i N(a_i^\dagger a_i) + \sum_{i \neq j} V_{ij} N(a_i^\dagger a_j) \quad (41)$$

$$= E_0(s=0) + \sum_{i=1}^3 e_i(s=0) N(a_i^\dagger a_i) + \sum_{i \neq j} g_{ij}(s=0) N(a_i^\dagger a_j) \quad (42)$$

Following the Wgner's choice,

$$\eta = [H^d, H^{od}] = \sum_{kl} (e_k - e_l) g_{kl} a_k^\dagger a_l \quad (43)$$

VII. FINITE SYSTEM

In finite system, \hat{g} is not diagonal since the translation invariance is not fulfilled. Several approximations for the generator in Eq. (24) have been tested and it is found that any approximation cannot give a convergent result. Some examples will be shown in the following subsections.

A. Generator I (similar to Nuclear Matter)

First, the generator which is analogous to Nuclear Matter is chosen,

$$\hat{\eta} = [\hat{g}, \hat{\Gamma}]. \quad (44)$$

Using Eq. (27a), (27b), this can be written as

$$\hat{\eta} = \hat{\eta}^{1b} + \hat{\eta}^{2b}. \quad (45)$$

Here one-body term shows up because the \hat{g} is not diagonal in general. Above generators are written as

$$\hat{\eta}^{1b} = \sum_{12} \eta_{12}^{1b} N(1^\dagger 2), \quad \hat{\eta}^{2b} = \frac{1}{4} \sum_{1234} \eta_{1234}^{2b} N(1^\dagger 2^\dagger 43), \quad (46)$$

where coefficients are defined as

$$\hat{\eta}_{12}^{1b} \equiv \sum_{ab} g_{ab} \Gamma_{b1a2} (n_a - n_b) \quad (47)$$

$$\hat{\eta}_{1234}^{2b} \equiv \sum_a (g_{1a} \Gamma_{a234} + g_{2a} \Gamma_{1a34} - g_{a3} \Gamma_{12a4} - g_{a4} \Gamma_{123a}) \quad (48)$$

One can see that these operators are anti-symmetric and anti-hermitian.

$$\eta_{12}^{1b} = -\eta_{21}^{1b}, \quad \eta_{1234}^{2b} = -\eta_{3412}^{2b} \quad (49)$$

$$\eta_{1234}^{2b} = -\eta_{2134}^{2b} = \eta_{2143}^{2b} = -\eta_{1243}^{2b}. \quad (50)$$

Now flow equation can be written as

$$\frac{d\hat{H}(s)}{ds} = [\hat{\eta}, \hat{H}(s)] = [\hat{\eta}^{1b} + \hat{\eta}^{2b}, \hat{g} + \hat{\Gamma}] \quad (51)$$

We calculate four individual terms of Eq. (50).

1. $[\hat{\eta}^{1b}, \hat{g}]$ part

This part, written as

$$[\hat{\eta}^{1b}, \hat{g}] = \sum_{12ab} \eta_{12}^{1b} g_{ab} [N(1^\dagger 2), N(a^\dagger b)], \quad (52)$$

gives one- and zero-body sectors.

$$[\hat{\eta}^{1b}, \hat{g}]_{1b} = \sum_{12} \sum_a (\eta_{1a}^{1b} g_{a2} - \eta_{a2}^{1b} g_{1a}) N(1^\dagger 2) \quad (53)$$

$$[\hat{\eta}^{1b}, \hat{g}]_{0b} = \sum_{12} \eta_{12}^{1b} g_{21} (n_1 - n_2) \quad (54)$$

2. $[\hat{\eta}^{1b}, \hat{\Gamma}]$ part

This part, written as

$$[\hat{\eta}^{1b}, \hat{\Gamma}] = \frac{1}{4} \sum_{1234ab} \eta_{ab}^{1b} \Gamma_{1234} [N(a^\dagger b), N(1^\dagger 2^\dagger 43)], \quad (55)$$

gives two- and one-body sectors.

$$[\hat{\eta}^{1b}, \hat{\Gamma}]_{2b} = \frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \sum_a (\eta_{1a}^{1b} \Gamma_{a234} + \eta_{2a}^{1b} \Gamma_{1a34} - \eta_{a3}^{1b} \Gamma_{12a4} - \eta_{a4}^{1b} \Gamma_{123a}) \quad (56)$$

$$\equiv \frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \underline{S_{1234}^{1b}} \quad (57)$$

$$[\hat{\eta}^{1b}, \hat{\Gamma}]_{1b} = \sum_{12} N(1^\dagger 2) \sum_{ab} \eta_{ab}^{1b} \Gamma_{b1a2} (n_a - n_b). \quad (58)$$

3. $[\hat{\eta}^{2b}, \hat{g}]$ part

This part, written as

$$[\hat{\eta}^{2b}, \hat{g}] = \frac{1}{4} \sum_{1234ab} \eta_{1234}^{2b} g_{ab} [N(1^\dagger 2^\dagger 43), N(a^\dagger b)], \quad (59)$$

gives two- and one-body sectors.

$$[\hat{\eta}^{2b}, \hat{g}]_{2b} = -\frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \sum_a [g_{1a} \eta_{a234}^{2b} + g_{2a} \eta_{1a34}^{2b} - g_{a3} \eta_{12a4}^{2b} - g_{a4} \eta_{123a}^{2b}] \quad (60)$$

$$\equiv -\frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \underline{S_{1234}^{2b}} \quad (61)$$

$$[\hat{\eta}^{2b}, \hat{g}]_{1b} = -\sum_{12} \sum_{ab} g_{ab} \eta_{b1a2}^{2b} (n_a - n_b) N(1^\dagger 2) \quad (62)$$

4. $[\hat{\eta}^{2b}, \hat{\Gamma}]$ part

This part, written as

$$[\hat{\eta}^{2b}, \hat{\Gamma}] = \frac{1}{16} \sum_{1234abcd} \eta_{1234}^{2b} \Gamma_{abcd} [N(1^\dagger 2^\dagger 43), N(a^\dagger b^\dagger dc)], \quad (63)$$

gives two- one- and zero-body sectors.

$$\begin{aligned}
[\hat{\eta}^{2b}, \hat{\Gamma}]_{2b} &= \frac{1}{4} \sum_{1234} \left[\frac{1}{2} \sum_{ab} (\eta_{12ab}^{2b} \Gamma_{ab34} - \eta_{ab34}^{2b} \Gamma_{12ab}) (1 - n_a - n_b) \right. \\
&\quad \left. - \sum_{ab} (n_a - n_b) \{ \eta_{b2a4}^{2b} \Gamma_{a1b3} - \eta_{a1b3}^{2b} \Gamma_{b2a4} + \eta_{a2b3}^{2b} \Gamma_{b1a4} - \eta_{b1a4}^{2b} \Gamma_{a2b3} \} \right] N(1^\dagger 2^\dagger 43)
\end{aligned} \tag{64}$$

$$[\hat{\eta}^{2b}, \hat{\Gamma}]_{1b} = \sum_{12} N(1^\dagger 2) \frac{1}{2} \left\{ \sum_{abc} (\eta_{c1ab}^{2b} \Gamma_{abc2} - \Gamma_{c1ab} \eta_{abc2}^{2b}) (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c) \right\} \tag{65}$$

$$[\hat{\eta}^{2b}, \hat{\Gamma}]_{0b} = \frac{1}{4} \sum_{1234} (\eta_{1234}^{2b} \Gamma_{3412} - \eta_{3412}^{2b} \Gamma_{1234}) n_1 n_2 \bar{n}_3 \bar{n}_4 \tag{66}$$

$$= \frac{1}{2} \sum_{1234} \eta_{1234}^{2b} \Gamma_{1234} n_1 n_2 \bar{n}_3 \bar{n}_4. \tag{67}$$

The hermisity of Γ_{1234} and the antihermisity of η_{1234} are used.

5. Flow equations in M -scheme formalism

Collecting all the terms, the flow equations are given as

$$\frac{d}{ds} E_0 = \sum_{12} \eta_{12}^{1b} g_{21} (n_1 - n_2) + \frac{1}{2} \sum_{1234} \eta_{1234}^{2b} \Gamma_{3412} n_1 n_2 \bar{n}_3 \bar{n}_4 \tag{68}$$

$$\begin{aligned}
\frac{d}{ds} g_{12} &= \sum_a (\eta_{1a}^{1b} g_{a2} - \eta_{a2}^{1b} g_{1a}) + \sum_{ab} \eta_{ab}^{1b} \Gamma_{b1a2} (n_a - n_b) \\
&\quad - \sum_{ab} g_{ab} \eta_{b1a2}^{2b} (n_a - n_b) + \frac{1}{2} \sum_{abc} (\eta_{c1ab}^{2b} \Gamma_{abc2} - \eta_{abc2}^{2b} \Gamma_{c1ab}) (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c)
\end{aligned} \tag{69}$$

$$\begin{aligned}
\frac{d\Gamma_{1234}}{ds} &= S_{1234}^{1b} - S_{1234}^{2b} + \frac{1}{2} \sum_{ab} (\eta_{12ab}^{2b} \Gamma_{ab34} - \eta_{ab34}^{2b} \Gamma_{12ab}) (1 - n_a - n_b) \\
&\quad - \sum_{ab} (n_a - n_b) \left\{ \underline{\eta}_{b2a4}^{2b} \Gamma_{a1b3} - \eta_{a1b3}^{2b} \Gamma_{b2a4} + \eta_{a2b3}^{2b} \Gamma_{b1a4} - \underline{\eta}_{b1a4}^{2b} \Gamma_{a2b3} \right\}
\end{aligned} \tag{70}$$

The last summation of Eq. (80) becomes the same as that of Scott when one replaces the dummy indices “a” and “b” in the terms with the underline.

6. Checking the results

We simply check the correctness of the result by just taking the limit of nuclear matter case, namely, $g_{ab} \rightarrow \delta_{ab}f_a$. In this case, the generators in Eq. (46) and (47) are given as

$$\eta_{12}^{1b} \rightarrow \sum_a f_a \Gamma_{a1a2} (n_a - n_a) = 0 \quad (71)$$

$$\eta_{1234}^{2b} = (f_1 + f_2 - f_3 - f_4) \Gamma_{1234} = (f_{12} - f_{34}) \Gamma_{1234}. \quad (72)$$

Thus, the first term of Eq. (78) vanishes and Eq. (78) becomes

$$\frac{dE_0}{ds} = \frac{1}{2} \sum_{1234} (f_{12} - f_{34}) |\Gamma_{1234}|^2 n_1 n_2 \bar{n}_3 \bar{n}_4. \quad (73)$$

This is the same as Eq. (35) of the nuclear matter case. In the same manner, one can show that all the flow equations go back to those of nuclear matter.

7. Numerical results

We show the results of the flow. The initial TBME's are V_{lowk} with $\Lambda = 2.0 fm^{-1}$ derived from av18 potential. The oscillator energy is $\hbar\omega = 14MeV$. The

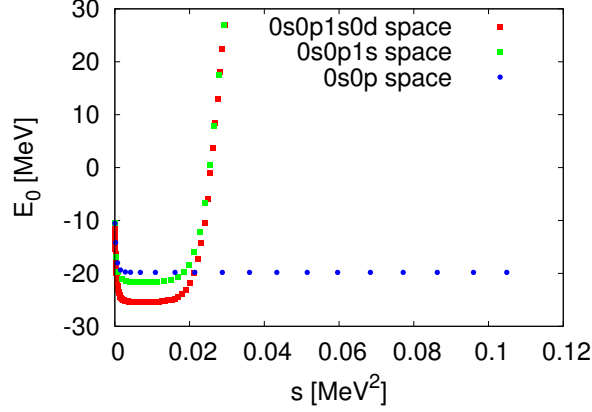


FIG. 1: The E_0 flow in sp, sps and spsd space.

B. Generator II (no approximation)

Unfortunately, the flow equations diverge if one chooses the generator of Eq. (43)

$$\hat{\eta} = [\hat{g}, \hat{\Gamma}], \quad \hat{H} = \hat{g} + \hat{\Gamma}. \quad (74)$$

Therefore we take another generator, following Wegner's choice in Eq. (24).

$$\hat{\eta} = [\hat{g}^d + \hat{\Gamma}^d, \hat{g}^{od} + \hat{\Gamma}^{od}]$$

The single-particle energies are defined according to the oscillator energies without spin-orbit splitting, $\epsilon_a = \epsilon_{n_a l_a j_a} = \hbar\omega(2n_a + l_a + 3/2)$. The generator is written as Using the commutation relations in Eqs. (27), the generator is obtained as

$$\hat{\eta} = \hat{\eta}^{1b} + \hat{\eta}^{2b} \quad (75)$$

$$\hat{\eta}^{1b} = \sum_{12} N(1^\dagger 2) \eta_{12}^{1b}, \quad \hat{\eta}^{1b} = \frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \eta_{1234}^{2b}, \quad (76)$$

where

$$\begin{aligned} \eta_{12}^{1b} = & \sum_a (g_{1a}^d g_{a2}^{od} - g_{1a}^{od} g_{a2}^d) - \sum_{ab} (n_a - n_b) g_{ab}^{od} \Gamma_{b1a2}^d \\ & + \frac{1}{2} \sum_{abc} (\Gamma_{c1ab}^d \Gamma_{abc2}^{od} - \Gamma_{c1ab}^{od} \Gamma_{abc2}^d) (\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) \end{aligned} \quad (77)$$

$$\begin{aligned} \eta_{1234}^{2b} = & \sum_a \{ (g_{1a}^d \Gamma_{a234}^{od} - g_{1a}^{od} \Gamma_{a234}^d) + (g_{2a}^d \Gamma_{1a34}^{od} - g_{2a}^{od} \Gamma_{1a34}^d) \\ & - (g_{a3}^d \Gamma_{12a4}^{od} - g_{a3}^{od} \Gamma_{12a4}^d) - (g_{a4}^d \Gamma_{123a}^{od} - g_{a4}^{od} \Gamma_{123a}^d) \} \\ & + \frac{1}{2} \sum_{ab} (\Gamma_{12ab}^d \Gamma_{ab34}^{od} - \Gamma_{12ab}^{od} \Gamma_{ab34}^d) (1 - n_a - n_b) \\ & + \sum_{ab} (n_a - n_b) (\Gamma_{b2a4}^d \Gamma_{a1b3} - \Gamma_{a1b3}^d \Gamma_{b2a4}^{od} + \Gamma_{a2b3}^d \Gamma_{b1a4}^{od} - \Gamma_{b1a4}^d \Gamma_{a2b3}^{od}) \end{aligned} \quad (78)$$

1. Flow equations in **M-scheme** formalism

Collecting all the terms, flow equations are given as

$$\frac{dE_0}{ds} = \sum_{12} \eta_{12}^{1b} g_{21}^{od} (n_1 - n_2) + \frac{1}{2} \sum_{1234} \eta_{1234}^{2b} \Gamma_{3412} n_1 n_2 \bar{n}_3 \bar{n}_4 \quad (79)$$

$$\begin{aligned} \frac{dg_{12}}{ds} = & \sum_a (\eta_{1a}^{1b} g_{a2} - \eta_{a2}^{1b} g_{1a}) + \sum_{ab} \eta_{ab}^{1b} \Gamma_{b1a2} (n_a - n_b) \\ & - \sum_{ab} g_{ab}^{od} \eta_{b1a2}^{2b} (n_a - n_b) + \frac{1}{2} \sum_{abc} (\eta_{c1ab}^{2b} \Gamma_{abc2} - \eta_{abc2}^{2b} \Gamma_{c1ab}) (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c) \end{aligned} \quad (80)$$

$$\begin{aligned} \frac{d\Gamma_{1234}}{ds} = & \sum_a (g_{1a} \eta_{a234}^{2b} + g_{2a} \eta_{1a34}^{2b} - g_{a3} \eta_{12a4}^{2b} - g_{a4} \eta_{123a}^{2b}) \\ & - \sum_a (g_{1a} \eta_{a234}^{2b} + g_{2a} \eta_{1a34}^{2b} - g_{a3} \eta_{12a4}^{2b} - g_{a4} \eta_{123a}^{2b}) \\ & + \frac{1}{2} \sum_{ab} (\eta_{12ab}^{2b} \Gamma_{ab34} - \eta_{ab34}^{2b} \Gamma_{12ab}) (1 - n_a - n_b) \\ & - \sum_{ab} (n_a - n_b) \{ \eta_{b2a4}^{2b} \Gamma_{a1b3} - \eta_{a1b3}^{2b} \Gamma_{b2a4} + \eta_{a2b3}^{2b} \Gamma_{b1a4} - \eta_{b1a4}^{2b} \Gamma_{a2b3} \} \end{aligned} \quad (81)$$

2. Flow equations in **jj-coupled** formalism

We just introduce the quantum numbers $k_a = (n_a, l_a, j_a, t_{za})$ and $\omega_a = (l_a, j_a, t_{za}, m_a)$. M-scheme matrix elements and J-scheme matrix elements are related as bellow

$$g_{12} = \delta_{m_1 m_2} g_{k_1 k_2}, \quad (g_{12} = \delta_{l_1 l_2} \delta_{j_1 j_2} \delta_{t_{z1} t_{z2}} \delta_{m_1 m_2} g_{12} = \delta_{l_1 l_2} \delta_{j_1 j_2} \delta_{t_{z1} t_{z2}} g_{k_1 k_2} = g_{k_1 k_2}) \quad (82)$$

$$\begin{aligned} \Gamma_{1234} &= \sqrt{(1 + \delta_{k_1 k_2})(1 + \delta_{k_3 k_4})} \sum_{JM} (j_1 m_1 j_2 m_2 | JM) (j_3 m_3 j_4 m_4 | JM) \Gamma_{k_1 k_2 k_3 k_4}^J \\ &\equiv \sum_{JM} (j_1 m_1 j_2 m_2 | JM) (j_3 m_3 j_4 m_4 | JM) \tilde{\Gamma}_{k_1 k_2 k_3 k_4}^J \end{aligned} \quad (83)$$

In the same way,

$$\eta_{12}^{1b} = \delta_{m_1 m_2} \eta_{k_1 k_2}^{1b} \quad (84)$$

$$\eta_{1234}^{2b} = \sum_{JM} (j_1 m_1 j_2 m_2 | JM) (j_3 m_3 j_4 m_4 | JM) \tilde{\eta}_{k_1 k_2 k_3 k_4}^{2b, J} \quad (85)$$

The generator is given by

$$\begin{aligned}
\eta_{k_1 k_2}^{1b} &= \sum_{k_a} (g_{k_1 k_a}^d g_{k_a k_2}^{od} - g_{k_1 k_a}^{od} g_{k_a k_2}^d) \\
&+ \frac{1}{(2j_1 + 1)} \sum_J (2J + 1) \left[- \sum_{k_a k_b} (n_a - n_b) g_{k_a k_b}^{od} \tilde{\Gamma}_{k_b k_1 k_a k_2}^{d,J} \right. \\
&+ \frac{1}{2} \sum_{k_a k_b k_c} \left(\tilde{\Gamma}_{k_c k_1 k_a k_b}^{d,J} \tilde{\Gamma}_{k_a k_b k_c k_2}^{od,J} - \tilde{\Gamma}_{k_c k_1 k_a k_b}^{od,J} \tilde{\Gamma}_{k_a k_b k_c k_2}^{d,J} \right) (\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) \left. \right] \quad (86) \\
\tilde{\eta}_{k_1 k_2 k_3 k_4}^{2b,J} &= \sum_{k_a} \left(g_{k_1 k_a}^d \tilde{\Gamma}_{k_a k_2 k_3 k_4}^{od,J} + g_{k_2 k_a}^d \tilde{\Gamma}_{k_1 k_a k_3 k_4}^{od,J} - g_{k_a k_3}^{d,1b} \tilde{\Gamma}_{k_1 k_2 k_a k_4}^{od,J} - g_{k_a k_4}^d \tilde{\Gamma}_{k_1 k_2 k_3 k_a}^{od,J} \right) \\
&- \sum_{k_a} \left(g_{k_1 k_a}^{od} \tilde{\Gamma}_{k_a k_2 k_3 k_4}^{d,J} + g_{k_2 k_a}^{od} \tilde{\Gamma}_{k_1 k_a k_3 k_4}^{d,J} - g_{k_a k_3}^{od} \tilde{\Gamma}_{k_1 k_2 k_a k_4}^{d,J} - g_{k_a k_4}^{od} \tilde{\Gamma}_{k_1 k_2 k_3 k_a}^{d,J} \right) \\
&+ \frac{1}{2} \sum_{k_a k_b} (1 - n_a - n_b) \left(\tilde{\Gamma}_{k_1 k_2 k_a k_b}^{d,J} \tilde{\Gamma}_{k_a k_b k_3 k_4}^{od,J} - \tilde{\Gamma}_{k_1 k_2 k_a k_b}^{od,J} \tilde{\Gamma}_{k_a k_b k_3 k_4}^{d,J} \right) \\
&- \sum_{k_a k_b} (n_a - n_b) \sum_{J_1 J_2} (2J_1 + 1)(2J_2 + 1)(-1)^{j_1 + j_3 + J_1 - J_2} \\
&\times \left[(-1)^J \begin{Bmatrix} j_a & j_4 & J_1 \\ j_1 & J & j_2 \\ J_2 & j_3 & j_b \end{Bmatrix} \left(\tilde{\Gamma}_{k_b k_2 k_a k_4}^{d,J_1} \tilde{\Gamma}_{k_a k_1 k_b k_3}^{od,J_2} - \tilde{\Gamma}_{k_b k_2 k_a k_4}^{od,J_1} \tilde{\Gamma}_{k_a k_1 k_b k_3}^{d,J_2} \right) \right. \\
&- \left. \begin{Bmatrix} j_a & j_4 & J_1 \\ j_2 & J & j_1 \\ J_2 & j_3 & j_b \end{Bmatrix} \left(\tilde{\Gamma}_{k_a k_2 k_b k_3}^{d,J_2} \tilde{\Gamma}_{k_b k_1 k_a k_4}^{od,J_1} - \tilde{\Gamma}_{k_a k_2 k_b k_3}^{od,J_2} \tilde{\Gamma}_{k_b k_1 k_a k_4}^{d,J_1} \right) \right] \quad (87)
\end{aligned}$$

In the J-scheme basis, the flow equations can be written as

$$\frac{d}{ds}E_0 = \frac{1}{2} \sum_{k_1 k_2 k_3 k_4} \sum_J (2J+1) \tilde{\eta}_{k_1 k_2 k_3 k_4}^{2b,J} \tilde{\Gamma}_{k_1 k_2 k_3 k_4}^{2b,J} n_1 n_2 \bar{n}_3 \bar{n}_4 + \sum_{k_1 k_2} (2j_1+1) \eta_{k_1 k_2}^{1b} g_{k_1 k_2}^{od} (n_1 - n_2) \quad (88)$$

$$\begin{aligned} \frac{d}{ds}g_{k_1 k_2} &= \sum_{k_a} (\eta_{k_1 k_a}^{1b} g_{k_a k_2} - g_{k_1 k_a} \eta_{k_a k_2}^{1b}) \\ &+ \frac{1}{(2j_1+1)} \sum_J (2J+1) \left[\sum_{k_a k_b} (n_a - n_b) \left\{ \eta_{k_a k_b}^{1b} \tilde{\Gamma}_{k_b k_1 k_a k_2}^J - g_{k_a k_b}^{od} \tilde{\eta}_{k_b k_1 k_a k_2}^{2b,J} \right\} \right. \\ &\left. \frac{1}{2} \sum_{k_a k_b k_c} \left(\tilde{\eta}_{k_c k_1 k_a k_b}^{2b,J} \tilde{\Gamma}_{k_a k_b k_c k_2}^J - \tilde{\Gamma}_{k_c k_1 k_a k_b}^J \tilde{\eta}_{k_a k_b k_c k_2}^{2b,J} \right) (\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) \right] \quad (89) \end{aligned}$$

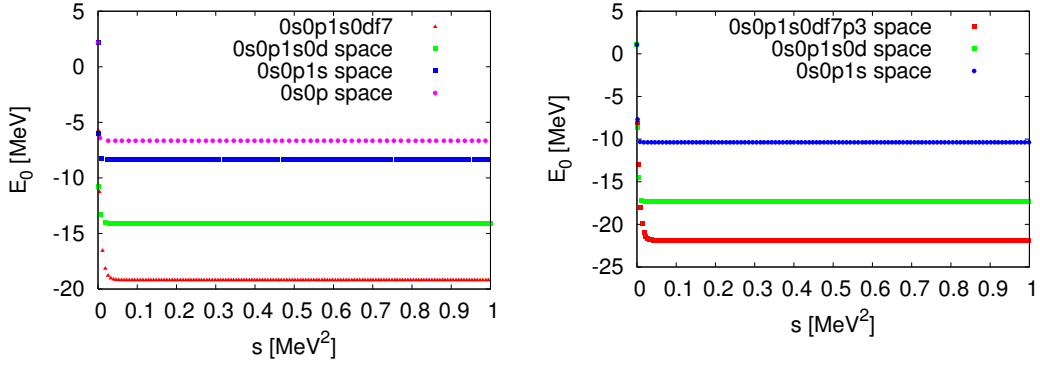
$$\begin{aligned} \frac{d}{ds} \tilde{\Gamma}_{k_1 k_2 k_3 k_4}^J &= \sum_{k_a} \left(\eta_{k_1 k_a}^{1b} \tilde{\Gamma}_{k_a k_2 k_3 k_4}^J + \eta_{k_2 k_a}^{1b} \tilde{\Gamma}_{k_1 k_a k_3 k_4}^J - \eta_{k_a k_3}^{1b} \tilde{\Gamma}_{k_1 k_2 k_a k_4}^J - \eta_{k_a k_4}^{1b} \tilde{\Gamma}_{k_1 k_2 k_3 k_a}^J \right) \\ &- \sum_{k_a} \left(g_{k_1 k_a} \tilde{\eta}_{k_a k_2 k_3 k_4}^{2b,J} + g_{k_2 k_a} \tilde{\eta}_{k_1 k_a k_3 k_4}^{2b,J} - g_{k_a k_3} \tilde{\eta}_{k_1 k_2 k_a k_4}^{2b,J} - g_{k_a k_4} \tilde{\eta}_{k_1 k_2 k_3 k_a}^{2b,J} \right) \\ &+ \frac{1}{2} \sum_{k_a k_b} (1 - n_a - n_b) \left(\tilde{\eta}_{k_1 k_2 k_a k_b}^{2b,J} \tilde{\Gamma}_{k_a k_b k_3 k_4}^J - \tilde{\Gamma}_{k_1 k_2 k_a k_b}^J \tilde{\eta}_{k_a k_b k_3 k_4}^{2b,J} \right) \\ &- \sum_{k_a k_b} (n_a - n_b) \sum_{J_1 J_2} (2J_1+1)(2J_2+1)(-1)^{j_1+j_3+J_1-J_2} \\ &\times \left[(-1)^J \begin{Bmatrix} j_a & j_4 & J_1 \\ j_1 & J & j_2 \\ J_2 & j_3 & j_b \end{Bmatrix} \left(\tilde{\eta}_{k_b k_2 k_a k_4}^{2b,J_1} \tilde{\Gamma}_{k_a k_1 k_b k_3}^{J_2} - \tilde{\Gamma}_{k_b k_2 k_a k_4}^{J_1} \tilde{\eta}_{k_a k_1 k_b k_3}^{2b,J_2} \right) \right. \\ &\left. - \begin{Bmatrix} j_a & j_4 & J_1 \\ j_2 & J & j_1 \\ J_2 & j_3 & j_b \end{Bmatrix} \left(\tilde{\eta}_{k_a k_2 k_b k_3}^{2b,J_2} \tilde{\Gamma}_{k_b k_1 k_a k_4}^{J_1} - \tilde{\Gamma}_{k_a k_2 k_b k_3}^{J_2} \tilde{\eta}_{k_b k_1 k_a k_4}^{2b,J_1} \right) \right] \quad (90) \end{aligned}$$

We have checked the M-scheme and jj-coupled flow equations show exactly the same results.

3. Numerical results

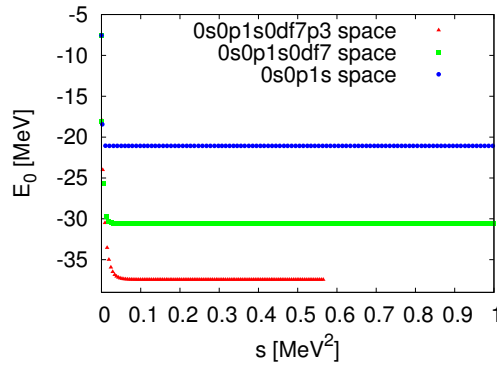
We use AV18 potential as NN potential which is renormalized to $V_{\text{low-k}}$ with several cutoff momentum Λ , then used as an initial Hamiltonian of the flow equations. We have checked that one- and two-body matrix elements have well converged and energetically off-diagonal matrix elements have become zero. The diagonal g_{ii} can be interpreted as the sum of the kinetic energy and self energy of the nucleon. Thus we consider g_{ii} as the single-particle energy of the nucleon ϵ_i . There are some cross-shell TBME's after the flow.

a. Assuming ^4He core In this case, the normal ordering is taken with respect to the ^4He core. First we show the E_0 flow with various initial inputs. The bigger space is needed for the flow equation.



(a) $\Lambda = 2.2 fm^{-1}, \hbar\omega = 16 \text{ MeV}$

(b) $\Lambda = 2.1 fm^{-1}, \hbar\omega = 18 \text{ MeV}$



(c) $\Lambda = 1.9 fm^{-1}, \hbar\omega = 16 \text{ MeV}$

FIG. 2: E_0 flow. The initial TBME's are V_{lowk} obtained from AV18 potential.

Next, we show the TBME's in $0p$ -shell obtained by the flow in sp sd space.

k_1	k_2	k_3	k_4	$2T_z$	$2J$	V	k_1	k_2	k_3	k_4	$2T_z$	$2J$	V
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	-2	0	-3.594445	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	2	-4.564122
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	-6.401160	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	-2.094314
$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	-0.100041	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	-2.481839
$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	2	1.320801	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	4	-1.541459
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	-2	4	-0.416260	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	0	4	-1.798661
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	4	-2.388369	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	4	1.791371
$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	4	-1.361456	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	0	4	-4.847598
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	0	-5.255744	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	0	4	-2.265166
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	0	0	-6.819774	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	4	-4.809090
$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	0	0	-1.489234	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	6	-5.624668
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	2	-2.204453	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	2	0	-4.968412
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	0	2	4.974673	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	2	0	-6.688591
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	2	-4.973483	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	2	0	-1.163374
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	2.238354	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	2	2	0.325695
$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	0	2	-4.618051	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	2	4	-1.530944
$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	0	2	5.000305	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	2	4	-2.488124
$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	2.105526	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	2	4	-2.486660

TABLE I: TBME's in $0p$ -shell. The initial TBME's are $V_{\text{low-k}}$ with $\Lambda=2.1\text{fm}^{-1}$, $\hbar\omega=18\text{MeV}$, from AV18. The flow equation was solved in sp sd-shell, assuming ^4He core. The S.P.E's are $\pi\epsilon_{0p3/2}=8.90$, $\nu\epsilon_{0p3/2}=6.53$, $\pi\epsilon_{0p1/2}=14.2$, $\nu\epsilon_{0p1/2}=11.9$

k_1	k_2	k_3	k_4	$2T_z$	$2J$	V	k_1	k_2	k_3	k_4	$2T_z$	$2J$	V
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	-2	0	-3.898173	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	2	-5.118363
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	-6.721788	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	-2.065114
$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	-0.509359	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	-2.992461
$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	2	1.421224	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	4	-1.580277
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	-2	4	-0.453570	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	0	4	-1.823027
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	4	-2.421618	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	4	1.815134
$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	4	-1.420647	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	0	4	-5.171379
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	0	-5.548650	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	0	4	-2.529495
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	0	0	-7.143991	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	4	-5.134294
$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	0	0	-1.864841	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	6	-6.161808
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	0	2	-2.788117	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	2	0	-5.267192
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	0	2	5.438401	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	2	0	-7.016472
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	0	2	-5.436474	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	2	0	-1.519731
$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	2.513046	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	2	2	0.418614
$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	0	2	-5.166887	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	2	4	-1.572467
$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	0	2	5.646205	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	2	4	-2.520769
$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	0	2	2.075184	$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	2	4	-2.546902

TABLE II: TBME's in $0p$ -shell. The initial TBME's are $V_{\text{low-k}}$ with $\Lambda=1.9\text{fm}^{-1}$, $\hbar\omega=16\text{MeV}$, from AV18. The flow equation was solved in $spsd$ -shell, assuming ^4He core. The S.P.E's are $\pi\epsilon_{0p3/2}=4.96$, $\nu\epsilon_{0p3/2}=2.50$, $\pi\epsilon_{0p1/2}=11.6$, $\nu\epsilon_{0p1/2}=9.25$

b. No-core case We also show the results of “No core” case. We have solved the flow equations without assuming any inert core. The evolved Hamiltonian can be used for the NCSM or other ab-initio method.

k_1	k_2	k_3	k_4	$2T_z$	$2J$	V	k_1	k_2	k_3	k_4	$2T_z$	$2J$	V
$0s_{1/2}$	$0s_{1/2}$	$0s_{1/2}$	$0s_{1/2}$	-2	0	-3.562298	$0p_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	-2.531795
$0s_{1/2}$	$0s_{1/2}$	$0s_{1/2}$	$1s_{1/2}$	-2	0	0	$0p_{3/2}$	$0p_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	-2	0	0
$0s_{1/2}$	$0s_{1/2}$	$0p_{3/2}$	$0p_{3/2}$	-2	0	0	$0p_{3/2}$	$0p_{3/2}$	$0d_{5/2}$	$0d_{5/2}$	-2	0	0
$0s_{1/2}$	$0s_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	0	$0p_{3/2}$	$0p_{3/2}$	$1s_{1/2}$	$1s_{1/2}$	-2	0	0
$0s_{1/2}$	$0s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	-2	0	0	$0p_{3/2}$	$0d_{3/2}$	$0p_{3/2}$	$0d_{3/2}$	-2	0	-0.753996
$0s_{1/2}$	$0s_{1/2}$	$0d_{5/2}$	$0d_{5/2}$	-2	0	0	$0p_{3/2}$	$0d_{3/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	0	-0.147864
$0s_{1/2}$	$0s_{1/2}$	$1s_{1/2}$	$1s_{1/2}$	-2	0	0	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	-0.175466
$0s_{1/2}$	$0p_{1/2}$	$0s_{1/2}$	$0p_{1/2}$	-2	0	-0.681605	$0p_{1/2}$	$0p_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	-2	0	0
$0s_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	$0d_{3/2}$	-2	0	0	$0p_{1/2}$	$0p_{1/2}$	$0d_{5/2}$	$0d_{5/2}$	-2	0	0
$0s_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	0	0	$0p_{1/2}$	$0p_{1/2}$	$1s_{1/2}$	$1s_{1/2}$	-2	0	0
$0s_{1/2}$	$1s_{1/2}$	$0s_{1/2}$	$1s_{1/2}$	-2	0	-5.614335	$0p_{1/2}$	$1s_{1/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	0	-1.038533
$0s_{1/2}$	$1s_{1/2}$	$0p_{3/2}$	$0p_{3/2}$	-2	0	-0.911573	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{3/2}$	-2	0	1.032993
$0s_{1/2}$	$1s_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	-2	0	0.400044	$0d_{3/2}$	$0d_{3/2}$	$0d_{5/2}$	$0d_{5/2}$	-2	0	-3.348263
$0s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	-2	0	0	$0d_{3/2}$	$0d_{3/2}$	$1s_{1/2}$	$1s_{1/2}$	-2	0	-0.017575
$0s_{1/2}$	$1s_{1/2}$	$0d_{5/2}$	$0d_{5/2}$	-2	0	0	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	-2	0	0.224703
$0s_{1/2}$	$1s_{1/2}$	$1s_{1/2}$	$1s_{1/2}$	-2	0	0	$0d_{5/2}$	$0d_{5/2}$	$1s_{1/2}$	$1s_{1/2}$	-2	0	0.061349
$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	-2	0	-1.474048	$1s_{1/2}$	$1s_{1/2}$	$1s_{1/2}$	$1s_{1/2}$	-2	0	-4.71741

TABLE III: TBME’s in *sp**sd*-shell. Only TBME’s with $J = 0, T_z = -1$ are listed. The initial TBME’s are $V_{\text{low-k}}$ with $\Lambda=2.2\text{fm}^{-1}$, $\hbar\omega=16\text{MeV}$, from AV18. The flow equation was solved in *sp**sd*-shell, assuming no core.

k_1	k_2	k_3	k_4	$2T_z$	$2J$	V	k_1	k_2	k_3	k_4	$2T_z$	$2J$	V
$0s_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	2	0	$0p_{3/2}$	$0d_{3/2}$	$0p_{3/2}$	$0d_{3/2}$	-2	2	0.927505
$0s_{1/2}$	$0p_{1/2}$	$0s_{1/2}$	$0p_{1/2}$	-2	2	-1.150871	$0p_{3/2}$	$0d_{3/2}$	$0p_{3/2}$	$0d_{5/2}$	-2	2	-0.803107
$0s_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	$0d_{3/2}$	-2	2	0	$0p_{3/2}$	$0d_{3/2}$	$0p_{3/2}$	$1s_{1/2}$	-2	2	0.106465
$0s_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	$0d_{5/2}$	-2	2	0	$0p_{3/2}$	$0d_{3/2}$	$0p_{1/2}$	$0d_{3/2}$	-2	2	-0.543598
$0s_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	$1s_{1/2}$	-2	2	0	$0p_{3/2}$	$0d_{3/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	2	0.731558
$0s_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$0d_{3/2}$	-2	2	0	$0p_{3/2}$	$0d_{5/2}$	$0p_{3/2}$	$0d_{5/2}$	-2	2	-0.853439
$0s_{1/2}$	$0p_{1/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	2	0	$0p_{3/2}$	$0d_{5/2}$	$0p_{3/2}$	$1s_{1/2}$	-2	2	-0.660307
$0s_{1/2}$	$0d_{3/2}$	$0s_{1/2}$	$0d_{3/2}$	-2	2	0.421124	$0p_{3/2}$	$0d_{5/2}$	$0p_{1/2}$	$0d_{3/2}$	-2	2	-2.812181
$0s_{1/2}$	$0d_{3/2}$	$0s_{1/2}$	$1s_{1/2}$	-2	2	0.948868	$0p_{3/2}$	$0d_{5/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	2	0.291229
$0s_{1/2}$	$0d_{3/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	2	-0.892203	$0p_{3/2}$	$1s_{1/2}$	$0p_{3/2}$	$1s_{1/2}$	-2	2	-0.518082
$0s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	$0d_{5/2}$	-2	2	0	$0p_{3/2}$	$1s_{1/2}$	$0p_{1/2}$	$0d_{3/2}$	-2	2	-0.263618
$0s_{1/2}$	$0d_{3/2}$	$0d_{3/2}$	$1s_{1/2}$	-2	2	0	$0p_{3/2}$	$1s_{1/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	2	2.068684
$0s_{1/2}$	$1s_{1/2}$	$0s_{1/2}$	$1s_{1/2}$	-2	2	0.646167	$0p_{1/2}$	$0d_{3/2}$	$0p_{1/2}$	$0d_{3/2}$	-2	2	0.583587
$0s_{1/2}$	$1s_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	2	-0.427519	$0p_{1/2}$	$0d_{3/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	2	-0.027257
$0s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{5/2}$	-2	2	0	$0p_{1/2}$	$1s_{1/2}$	$0p_{1/2}$	$1s_{1/2}$	-2	2	0.660167
$0s_{1/2}$	$1s_{1/2}$	$0d_{3/2}$	$1s_{1/2}$	-2	2	0	$0d_{3/2}$	$0d_{5/2}$	$0d_{3/2}$	$0d_{5/2}$	-2	2	0.539495
$0p_{3/2}$	$0p_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	-2	2	0.166944	$0d_{3/2}$	$0d_{5/2}$	$0d_{3/2}$	$1s_{1/2}$	-2	2	0.344692
$0p_{3/2}$	$0p_{1/2}$	$0d_{3/2}$	$0d_{5/2}$	-2	2	0	$0d_{3/2}$	$1s_{1/2}$	$0d_{3/2}$	$1s_{1/2}$	-2	2	0.659177
$0p_{3/2}$	$0p_{1/2}$	$0d_{3/2}$	$1s_{1/2}$	-2	2	0							

TABLE IV: TBME's in *spsd*-shell. Only TBME's with $J = 1, T_z = -1$ are listed. The initial TBME's are $V_{\text{low-k}}$ with $\Lambda=2.2\text{fm}^{-1}$, $\hbar\omega=16\text{MeV}$, from AV18. The flow equation was solved in *spsd*-shell, assuming no core.

C. Generator III

We introduce the projection operator P_i ($i = 1, \dots, N$)

$$\sum_i P_i = 1, \quad P_i P_j = P_i \delta_{ij}. \quad (91)$$

One can then split a Hamiltonian

$$H = \sum_i P_i H P_i + \sum_{i \neq j} P_i H P_j \quad (92)$$

$$= H_d + H_{od}. \quad (93)$$

We are testing this choice numerically.

APPENDIX A: THE PROOF OF THE FUNDAMENTAL COMMUTATORS

1. The proof of $[\hat{A}^{1b}, \hat{B}^{2b}]_{2b}$

This sector contains one contraction.

$$[N(a^\dagger b), N(1^\dagger 2^\dagger 43)]_{2b} = N(a^\dagger b)N(1^\dagger 2^\dagger 43) - N(1^\dagger 2^\dagger 43)N(a^\dagger b)|_{2b} \quad (A1)$$

$$\begin{aligned} &= \delta_{a3}n_3N(b1^\dagger 2^\dagger 4) - \delta_{a3}\bar{n}_3N(1^\dagger 2^\dagger 4b) - \delta_{a4}n_4N(b1^\dagger 2^\dagger 3) + \delta_{a4}\bar{n}_4N(1^\dagger 2^\dagger 3b) \\ &+ \delta_{b1}n_1N(a^\dagger 2^\dagger 43) - \delta_{b1}\bar{n}_1N(2^\dagger 43a^\dagger) - \delta_{b2}n_2N(a^\dagger 1^\dagger 43) + \delta_{b2}\bar{n}_2N(1^\dagger 43a^\dagger) \end{aligned} \quad (A2)$$

Using this relation, one obtains the 2b sector of the commutator as

$$\begin{aligned} [\hat{A}^{1b}, \hat{B}^{2b}]_{2b} &= \frac{1}{4} \sum_{ab} \sum_{1234} A_{ab} B_{1234} [N(a^\dagger b), N(1^\dagger 2^\dagger 43)]_{2b} \\ &= -\frac{1}{4} \sum_{b1234} A_{3b} B_{1234} (n_3 + \bar{n}_3) N(1^\dagger 2^\dagger 4b) - \frac{1}{4} \sum_{b1234} A_{3b} B_{1234} (n_4 + \bar{n}_4) N(1^\dagger 2^\dagger b3) \end{aligned} \quad (A3)$$

$$\begin{aligned} &= -\frac{1}{4} \sum_{b1234} A_{3b} B_{1234} (n_3 + \bar{n}_3) N(1^\dagger 2^\dagger 4b) - \frac{1}{4} \sum_{b1234} A_{3b} B_{1234} (n_4 + \bar{n}_4) N(1^\dagger 2^\dagger b3) \\ &+ \frac{1}{4} \sum_{a1234} N(a^\dagger 2^\dagger 43) A_{a1} B_{1234} (n_1 + \bar{n}_1) + \frac{1}{4} \sum_{a1234} N(1^\dagger a^\dagger 43) A_{a2} B_{1234} (n_2 + \bar{n}_2) \end{aligned} \quad (A4)$$

$$= \frac{1}{4} \sum_{a1234} N(1^\dagger 2^\dagger 43) [-A_{a3} B_{12a4} - A_{a4} B_{123a} + A_{1a} B_{a234} + A_{2a} B_{1a34}] \quad (A5)$$

$$= \frac{1}{4} \sum_{1234} N(a^\dagger 2^\dagger 43) \sum_a \{A_{1a} B_{a234} + A_{2a} B_{1a34} - A_{a3} B_{12a4} - A_{a4} B_{123a}\}. \quad (A6)$$

From Eq. (A4) to Eq. (A5), indices of the four terms in Eq. (A4) are replaced as

$$\begin{aligned} \text{1st} : b &\rightarrow 3, 3 \rightarrow a & \text{2nd} : b &\rightarrow 4, 4 \rightarrow a \\ \text{3rd} : a &\leftrightarrow 1 & \text{2nd} : a &\leftrightarrow 2 \end{aligned}$$

2. The proof of $[\hat{A}^{1b}, \hat{B}^{2b}]_{1b}$

This sector contains two contractions.

$$[N(a^\dagger b), N(1^\dagger 2^\dagger 43)]_{1b} = N(a^\dagger b)N(1^\dagger 2^\dagger 43) - N(1^\dagger 2^\dagger 43)N(a^\dagger b)|_{1b} \quad (A7)$$

$$\begin{aligned} &= \delta_{a3}\delta_{b1} (n_3\bar{n}_1 - \bar{n}_3n_1) N(2^\dagger 4) - \delta_{a3}\delta_{b2} (n_3\bar{n}_2 - \bar{n}_3n_2) N(1^\dagger 4) \\ &- \delta_{a4}\delta_{b1} (n_4\bar{n}_1 - \bar{n}_4n_1) N(2^\dagger 3) + \delta_{a4}\delta_{b2} (n_4\bar{n}_2 - \bar{n}_4n_2) N(1^\dagger 3) \end{aligned} \quad (A8)$$

Using this commutation relation, the one-body sector of the commutator is written as

$$[\hat{A}^{1b}, \hat{B}^{2b}]_{1b} = \frac{1}{4} \sum_{ab} \sum_{1234} A_{ab} B_{1234} [N(a^\dagger b), N(1^\dagger 2^\dagger 43)]_{1b} \quad (\text{A9})$$

$$\begin{aligned} &= \frac{1}{4} \sum_{1234} N(2^\dagger 4) A_{31} B_{1234} (n_3 - n_1) - \frac{1}{4} \sum_{1234} N(1^\dagger 4) A_{32} B_{1234} (n_3 - n_2) \\ &\quad - \frac{1}{4} \sum_{1234} N(2^\dagger 3) A_{41} B_{1234} (n_4 - n_1) + \frac{1}{4} \sum_{1234} N(1^\dagger 3) A_{42} B_{1234} (n_4 - n_2) \end{aligned} \quad (\text{A10})$$

Replacing indices of Eq. (A10) as

$$\begin{aligned} \text{1st} : (1, 2, 3, 4) &\rightarrow (b, 1, a, 2) & \text{2nd} : (2, 3, 4) &\rightarrow (b, a, 2) \\ \text{3rd} : (1, 2, 3, 4) &\rightarrow (b, 1, 2, a) & \text{2nd} : (2, 3, 4) &\rightarrow (b, 2, a) \end{aligned}$$

one can reach

$$\begin{aligned} [\hat{A}^{1b}, \hat{B}^{2b}]_{1b} &= \frac{1}{4} \sum_{12} N(1^\dagger 2) \sum_{ab} 4A_{ab} B_{b1a2} (n_a - n_b) \\ &= \sum_{12} N(1^\dagger 2) \sum_{ab} A_{ab} B_{b1a2} (n_a - n_b) \end{aligned} \quad (\text{A11})$$

3. The proof of $[\hat{A}^{1b}, \hat{B}^{1b}]_{0,1b}$

Following the relation

$$\begin{aligned} [N(1^\dagger 2), N(a^\dagger b)] &= \delta_{1b} \delta_{2a} n_1 \bar{n}_2 - \delta_{1b} \delta_{2a} \bar{n}_1 n_2 \\ &\quad + \delta_{1b} (n_1 N(2a^\dagger) - \bar{n}_1 N(a^\dagger 2)) + \delta_{2a} (\bar{n}_2 N(1^\dagger b) - n_2 N(b1^\dagger)) \\ &= \delta_{1b} \delta_{2a} n_1 \bar{n}_2 - \delta_{1b} \delta_{2a} \bar{n}_1 n_2 - \delta_{1b} N(a^\dagger 2) + \delta_{2a} N(1^\dagger b), \end{aligned} \quad (\text{A12})$$

one obtains the contributions

$$\begin{aligned} [\hat{A}^{1b}, \hat{B}^{1b}]_{1b} &= - \sum_{12} \sum_a A_{12} B_{a1} N(a^\dagger 2) + \sum_{12} \sum_b A_{12} B_{2b} N(1^\dagger b) \\ &= \sum_{12} N(1^\dagger 2) \sum_a (A_{1a} B_{a2} - B_{1a} A_{a2}) \end{aligned} \quad (\text{A13})$$

$$\begin{aligned} [\hat{A}^{1b}, \hat{B}^{1b}]_{0b} &= \sum_{12} A_{12} B_{21} n_1 \bar{n}_2 - \sum_{12} A_{12} B_{21} \bar{n}_1 n_2 \\ &= \sum_{12} A_{12} B_{21} (n_1 - n_2) \end{aligned} \quad (\text{A14})$$

4. The proof of $[\hat{A}^{2b}, \hat{B}^{2b}]_{2b}$

The commutator

$$[N(1^\dagger 2^\dagger 43), N(a^\dagger b^\dagger dc)]_{2b} = \{N(1^\dagger 2^\dagger 43)N(a^\dagger b^\dagger dc) - N(a^\dagger b^\dagger dc)N(1^\dagger 2^\dagger 43)\}_{2b} \quad (\text{A15})$$

is divided into two groups. One is

$$N(\overline{1^\dagger 2^\dagger 43})N(\overline{a^\dagger b^\dagger dc}), \quad N(1^\dagger 2^\dagger \overline{43})N(\overline{a^\dagger b^\dagger dc}). \quad (\text{A16})$$

Two creation (annihilation) operators in the left normal-ordering contract with the two annihilation (creation) operators in the right normal-ordering. We will denote this group as “X”.

The other one is

$$N(\overline{1^\dagger 2^\dagger 43})N(\overline{a^\dagger b^\dagger dc}), \quad (\text{A17})$$

that is, creation and annihilation operators in the left normal-ordering contract with annihilation and creation operators in the right normal-ordering, respectively. We will call this group “Y”.

c. Group X Terms which belong to the group X are

$$\begin{aligned} & [N(1^\dagger 2^\dagger 43), N(a^\dagger b^\dagger dc)]_{2b, \text{group-X}} \\ &= \delta_{1c}\delta_{2d}n_1n_2N(43a^\dagger b^\dagger) - \delta_{1c}\delta_{2d}\bar{n}_1\bar{n}_2N(a^\dagger b^\dagger 43) - \delta_{1d}\delta_{2c}n_1n_2N(43a^\dagger b^\dagger) + \delta_{1d}\delta_{2c}\bar{n}_1\bar{n}_2N(a^\dagger b^\dagger 43) \\ &= \delta_{3a}\delta_{4b}\bar{n}_3\bar{n}_2N(1^\dagger 2^\dagger dc) - \delta_{3a}\delta_{4b}n_3n_4N(dc1^\dagger 2^\dagger) - \delta_{3b}\delta_{4a}\bar{n}_3\bar{n}_4N(1^\dagger 2^\dagger dc) + \delta_{4a}\delta_{3b}n_3n_4N(dc1^\dagger 2^\dagger) \end{aligned} \quad (\text{A18})$$

With the anti-symmetric properties of A_{1234}^{2b} and B_{abcd}^{2b} , the contribution from the group X is

$$\begin{aligned}
[\hat{A}^{2b}, \hat{B}^{2b}]|_{2b, group-X} &= \frac{2}{16} \sum_{1234} \sum_{abcd} A_{1234} B_{abcd} [\delta_{1c} \delta_{2d} (n_1 n_2 - \bar{n}_1 \bar{n}_2) N(a^\dagger b^\dagger 43) \\
&\quad + \delta_{3a} \delta_{4b} (\bar{n}_3 \bar{n}_4 - n_3 n_4) N(1^\dagger 2^\dagger dc)] \\
&= \frac{1}{8} \sum_{1234} \sum_{ab} A_{1234} B_{ab12} (n_1 + n_2 - 1) N(a^\dagger b^\dagger 43) \\
&\quad + \frac{1}{8} \sum_{1234} \sum_{cd} A_{1234} B_{34cd} (1 - n_3 + n_4) N(1^\dagger 2^\dagger dc) \\
&= \frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \left\{ \frac{1}{2} \sum_{ab} (A_{ab34} B_{12ab} - B_{ab34} A_{12ab}) (1 - n_a - n_b) \right\}.
\end{aligned} \tag{A19}$$

d. Group Y Terms which belong to the group Y are

$$\begin{aligned}
&[N(1^\dagger 2^\dagger 43), N(a^\dagger b^\dagger dc)]|_{2b, group-B} \\
&= \delta_{1c} \delta_{3a} n_1 \bar{n}_3 N(2^\dagger 4b^\dagger d) - \delta_{1c} \delta_{3a} \bar{n}_1 n_3 N(b^\dagger d 2^\dagger 4) - \delta_{1c} \delta_{3b} n_1 \bar{n}_3 N(2^\dagger 4a^\dagger d) + \delta_{1c} \delta_{3b} \bar{n}_1 n_3 N(a^\dagger d 2^\dagger 4) \\
&\quad - \delta_{1d} \delta_{3a} n_1 \bar{n}_3 N(2^\dagger 4b^\dagger c) + \delta_{1d} \delta_{3a} \bar{n}_1 n_3 N(b^\dagger c 2^\dagger 4) + \delta_{1d} \delta_{3b} n_1 \bar{n}_3 N(2^\dagger 4a^\dagger c) - \delta_{1d} \delta_{3b} \bar{n}_1 n_3 N(a^\dagger c 2^\dagger 4)
\end{aligned} \tag{A20a}$$

$[(1^\dagger, 3)$ are contracted with other operators $(a^\dagger, b^\dagger c, d)]$

$$+ [(1^\dagger, 3) \rightarrow (1^\dagger, 4)] \tag{A20b}$$

$$+ [(1^\dagger, 3) \rightarrow (2^\dagger, 3)] \tag{A20c}$$

$$+ [(1^\dagger, 3) \rightarrow (2^\dagger, 4)] \tag{A20d}$$

From Eqs. (A20), one obtains the commutations, respectively

$$\begin{aligned}
&-\frac{4}{16} \sum_{1234} \sum_{bd} n_1 \bar{n}_3 N(2^\dagger b^\dagger 4d) + \frac{4}{16} \sum_{1234} \sum_{bd} \bar{n}_1 n_3 N(2^\dagger b^\dagger 4d) \\
&= \frac{1}{4} \sum_{1234} \sum_{bd} (n_3 - n_1) A_{1234} B_{3b1d} N(2^\dagger b^\dagger 4d),
\end{aligned} \tag{A21a}$$

$$\frac{1}{4} \sum_{1234} \sum_{bd} (n_4 - n_1) A_{1234} B_{b41d} N(2^\dagger b^\dagger 3d), \tag{A21b}$$

$$\frac{1}{4} \sum_{1234} \sum_{bd} (n_3 - n_2) A_{1234} B_{3bd2} N(1^\dagger b^\dagger 4d), \tag{A21c}$$

$$\frac{1}{4} \sum_{1234} \sum_{bd} (n_4 - n_2) A_{1234} B_{4b2d} N(1^\dagger b^\dagger 3d). \tag{A21d}$$

Changing the dummy indices, the contribution from the group Y is

$$[\hat{A}^{2b}, \hat{B}^{2b}]_{2b, group-Y} = \frac{1}{4} \sum_{1234} N(1^\dagger 2^\dagger 43) \times \left\{ \sum_{ab} (n_a - n_b) (A_{a1b3} B_{b2a4} - A_{a2b3} B_{b1a4} - A_{a1b4} B_{b2a3} + A_{a2b4} B_{b1a3}) \right\} \quad (A22)$$

Summing up Eq. (A19) and (A22), one obtains Eq. (27e)

5. The proof of $[\hat{A}^{2b}, \hat{B}^{2b}]_{1b}$

In this case, there are three contractions between the left and the right normal-ordering. Each terms can be characterized by the creation and annihilation operators which are kept unchanged without any contraction. There are two types of contractions.

One is the type that an annihilation operator in the left normal-ordering and a creation operator in the right normal-ordering are left.

$$N(\overbrace{1^\dagger 2^\dagger 43}) \overbrace{N(a^\dagger b^\dagger dc)} \quad (A23)$$

In this case, $(4, b^\dagger)$ are left. There are four terms like this, and for each term, there are two possibilities of the contraction between $(1^\dagger, 2^\dagger)$ and (c, d) . Thus, in total, one has eight terms from this type of contraction, where every terms give the same contributions. Therefore, one obtains

$$-8 \times \frac{1}{16} \sum_{1234} \sum_a A_{1234} B_{3a12} (n_1 n_2 \bar{n}_3 + \bar{n}_1 \bar{n}_3 n_3) N(a^\dagger 4). \quad (A24)$$

The other one is

$$N(\overbrace{1^\dagger 2^\dagger 43}) \overbrace{N(a^\dagger b^\dagger dc)}. \quad (A25)$$

This is the case that a creation operator in the left normal-ordering and an annihilation operator in the right normal-ordering are left. There are also eight terms, giving the same contribution. One gets

$$8 \times \frac{1}{16} \sum_{1234} \sum_a A_{1234} B_{34a2} (n_3 n_4 \bar{n}_2 + \bar{n}_3 \bar{n}_4 n_2) N(1^\dagger a). \quad (A26)$$

Replacing the dummy indices in Eq. (A24) and (A26), one finally obtains

$$[\hat{A}^{2b}, \hat{B}^{2b}]_{1b} = \sum_{12} N(1^\dagger 2) \left\{ \frac{1}{2} \sum_{abc} (A_{1cab} B_{ab2c} - B_{1cab} A_{abc2}) (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c) \right\} \quad (A27)$$

6. The proof of $[\hat{A}^{2b}, \hat{B}^{2b}]_{0b}$

In this case, all operators are contracted

$$[\hat{A}^{2b}, \hat{B}^{2b}]_{0b} = \frac{1}{16} \sum_{1234} \sum_{abcd} A_{1234} B_{abcd} [N(1^\dagger 2^\dagger 43), N(a^\dagger b^\dagger dc)]_{0b} \quad (\text{A28})$$

$$\begin{aligned} [N(1^\dagger 2^\dagger 43), N(a^\dagger b^\dagger dc)]_{0b} &= N(\overbrace{1^\dagger 2^\dagger 43}^{\text{---}} \overbrace{a^\dagger b^\dagger dc}^{\text{---}}) - N(\overbrace{a^\dagger b^\dagger dc}^{\text{---}} \overbrace{1^\dagger 2^\dagger 43}^{\text{---}}) \\ &\quad + (4 \text{ terms by permutation}) - (4 \text{ terms by permutation}). \end{aligned} \quad (\text{A29})$$

Thus,

$$[\hat{A}^{2b}, \hat{B}^{2b}]_{0b} = \frac{1}{4} \sum_{1234} A_{1234} B_{3412} (n_1 n_2 \bar{n}_3 \bar{n}_4 - \bar{n}_1 \bar{n}_2 n_3 n_4) \quad (\text{A30})$$

$$= \frac{1}{4} \sum_{1234} (A_{1234} B_{3412} - B_{1234} A_{3412}) n_1 n_2 \bar{n}_3 \bar{n}_4 \quad (\text{A31})$$