

- Derivation for SRG evolved overlap

$$\langle \psi_{\alpha}^{A-1} | \hat{U}_{\lambda}^{\dagger} \hat{U}_{\lambda} a_{\vec{p}} \hat{U}_{\lambda}^{\dagger} \hat{U}_{\lambda} | \psi_0^A \rangle \quad (1)$$

where α is specified by $\{n, j, l, s, \tau\}$.

i) $a_{\vec{p}}$ must have some spin and isospin projection:

$$a_{\vec{p}} \rightarrow a_{\vec{p}\sigma\tau}$$

$$\text{ii) } \hat{U}_{\lambda} | \psi_0^A \rangle = | \psi_0^A(\lambda) \rangle \equiv | \mathbb{E} \rangle \quad (2)$$

$$\text{iii) } \langle \psi_{\alpha}^{A-1} | \hat{U}_{\lambda}^{\dagger} = \langle \psi_{\alpha}^{A-1}(\lambda) |$$

$$= \langle \psi_0^A(\lambda) | a_{\alpha}^{\dagger}$$

$$= \langle \mathbb{E} | a_{\alpha}^{\dagger} \quad (3)$$

Then Eq. (1) reads

$$\langle \mathbb{E} | a_{\alpha}^{\dagger} \hat{U}_{\lambda} a_{\vec{p}\sigma\tau} \hat{U}_{\lambda}^{\dagger} | \mathbb{E} \rangle \quad (4)$$

(2)

The strategy is to evaluate $a_\alpha^\dagger \hat{U}_\lambda a_{\vec{p}\sigma z} \hat{U}_\lambda^\dagger$
at the 2-body level using the expansion of \hat{U}_λ :

$$\hat{U}_\lambda = \hat{I} + \frac{1}{4} \sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \sum_{z_1 z_2 z_3 z_4} \sum_{\vec{k} \vec{k}'} \langle \vec{k} \sigma_1 z_1 \vec{k}' \sigma_2 z_2 | \delta \hat{U} | \vec{k}' \sigma_3 z_3 \vec{k} \sigma_4 z_4 \rangle$$

$$\times a_{\vec{k}+\vec{k}'}^\dagger \sigma_1 \tau_1 a_{\vec{k}-\vec{k}'}^\dagger \sigma_2 \tau_2 a_{\vec{k}-\vec{k}'} \sigma_3 \tau_3 a_{\vec{k}+\vec{k}'} \sigma_4 \tau_4 + \dots \quad (5)$$

where $\delta \hat{U} = (1 - \hat{P}_{12}) \delta U$

The only terms that are less than 3-body are given below

$$\text{I)} \quad a_\alpha^\dagger \hat{I} a_{\vec{p}\sigma z} \hat{I}$$

$$\text{II)} \quad a_\alpha^\dagger \hat{I} a_{\vec{p}\sigma z} \delta \hat{U}^\dagger$$

Start with I):

Using $a_i = \sum_j \langle i | j \rangle a_j$ we can write

$a_{\vec{p}\sigma z}$ in terms of single-particle (s.p.) states β
(these will be indicated by Greek letters):

$$a_{\vec{p}\sigma z} = \sum_\beta \langle \vec{p}\sigma z | \beta \rangle a_\beta \quad (6)$$

$$\text{where } \langle \vec{p} \sigma \epsilon | \beta \rangle = \Phi_\beta(|\vec{p}|) Y_{\ell'}^{m'}(\Omega_{\vec{p}}) \langle \ell' m' s \sigma | j' m_j' \rangle \quad (5)$$

and $m_\ell' = m_j' - \sigma$ and $s = \frac{1}{2}$. Then Eq. (6) reads

$$a_{\vec{p} \sigma \epsilon} = \sum_\beta \Phi_\beta(p) Y_{\ell'}^{m_j' - \sigma}(\Omega_{\vec{p}}) \langle \ell' m_j' - \sigma \frac{1}{2} \sigma | j' m_j' \rangle a_\beta \quad (7)$$

We will use Eq. (7) to also transform the creation and annihilation operators of \hat{U}_1^+ later.

Now for the $a_\alpha^\dagger \hat{I} a_{\vec{p} \sigma \epsilon} \hat{I}$ term we have

$$\sum_\beta \Phi_\beta(p) Y_{\ell'}^{m_j' - \sigma}(\Omega_{\vec{p}}) \langle \ell' m_j' - \sigma \frac{1}{2} \sigma | j' m_j' \rangle a_\alpha^\dagger a_\beta \quad (8)$$

This is a 1-body operator. Diagrammatically

$$\alpha \quad \underbrace{\quad \quad \quad}_\beta$$

For Π , we start by transforming the creation and annihilation operators to the s.p. basis

$$\Rightarrow \frac{1}{4} \sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \sum_{\tau_1 \tau_2 \tau_3 \tau_4} \sum_{\vec{k} \vec{k}' \vec{k}''} \langle \vec{k} \sigma_1 \tau_1 \sigma_2 \tau_2 | \delta \tilde{U}^+ | \vec{k}' \sigma_3 \tau_3 \vec{k}'' \sigma_4 \tau_4 \rangle \\ \times \sum_{\rho \sigma \mu \nu} \Phi_\rho(|\vec{k}_\perp + \vec{k}|) \Phi_\sigma^*(|\vec{k}_\perp - \vec{k}|) \Phi_\mu(|\vec{k}_\perp + \vec{k}'|) \Phi_\nu(|\vec{k}_\perp - \vec{k}'|)$$

$$\begin{aligned}
 & \times Y_{l_1}^{m_{j_1}-\sigma_1}(\Omega_{\vec{k}+\vec{k}}) Y_{l_2}^{m_{j_2}-\sigma_2}(\Omega_{\vec{k}-\vec{k}}) Y_{l_3}^{m_{j_3}-\sigma_3}(\Omega_{\vec{k}+\vec{k}'}) Y_{l_4}^{m_{j_4}-\sigma_4}(\Omega_{\vec{k}-\vec{k}'}) \\
 & \times \langle j_1 m_{j_1} | l_1 m_{j_1} \sigma_1 \pm \sigma_1 \rangle \langle j_2 m_{j_2} | l_2 m_{j_2} \sigma_2 \pm \sigma_2 \rangle \langle l_3 m_{j_3} \sigma_3 \pm \sigma_3 | j_3 m_{j_3} \rangle \\
 & \times \langle l_4 m_{j_4} \sigma_4 \pm \sigma_4 | j_4 m_{j_4} \rangle a_\alpha^\dagger a_\beta a_\rho^\dagger a_\sigma^\dagger a_\nu a_\mu
 \end{aligned} \tag{9}$$

Applying Wick's theorem :

$$a_\alpha^\dagger a_\beta a_\rho^\dagger a_\sigma^\dagger a_\nu a_\mu = :a_\alpha^\dagger a_\beta a_\rho^\dagger a_\sigma^\dagger a_\nu a_\mu: \quad \text{3-body}$$

$$+ :a_\alpha^\dagger a_\beta a_\rho^\dagger a_\sigma^\dagger a_\nu a_\mu:$$

$$- :a_\alpha^\dagger a_\beta a_\rho^\dagger a_\sigma^\dagger a_\nu a_\mu:$$

$$\alpha \begin{array}{c} \uparrow \\ \boxed{\text{set}} \\ \downarrow \end{array} \mu$$

$$\mu \begin{array}{c} \uparrow \\ \boxed{\text{set}} \\ \downarrow \end{array} \nu$$

$$= \delta_{\beta\rho} a_\alpha^\dagger a_\sigma^\dagger a_\nu a_\mu - \delta_{\rho\sigma} a_\alpha^\dagger a_\rho^\dagger a_\nu a_\mu \tag{10}$$

Next we evaluate matrix elements with respect to $|\mathbb{E}\rangle$ assuming $|\mathbb{E}\rangle$ is given by independent-particle model :

$$|\mathbb{E}\rangle = \prod_{\alpha \text{ occupied}} a_\alpha^\dagger |0\rangle \tag{11}$$

Focusing only on the creation and annihilation operators

$$I) \quad \langle \mathbb{E} | a_\alpha^\dagger a_\beta | \mathbb{E} \rangle = \delta_{\alpha\beta} \tag{12}$$

(5)

$$\text{and II) } \langle \Phi | [\delta_{\beta\mu} a_\alpha^\dagger a_\sigma^\dagger a_\nu a_\mu - \delta_{\beta\sigma} a_\alpha^\dagger a_\rho^\dagger a_\nu a_\mu] | \Phi \rangle$$

$$= \delta_{\beta\mu} (\delta_{\alpha\mu} \delta_{\sigma\nu} - \delta_{\alpha\nu} \delta_{\sigma\mu}) - \delta_{\beta\sigma} (\delta_{\alpha\mu} \delta_{\rho\nu} - \delta_{\alpha\nu} \delta_{\rho\mu}) \quad (13)$$

Combine all equations to find

$$\langle \Phi | a_\alpha^\dagger \hat{U}_\lambda a_{\vec{p}\sigma z} \hat{U}_\lambda^\dagger | \Phi \rangle$$

$$= \sum_{\beta} \phi_{\beta}(\rho) \gamma_{\ell', j'-\sigma}^{m_j'-\sigma}(\Omega_{\vec{p}}) \langle \ell' m_j'-\sigma \pm \sigma | j' m_j' \rangle \delta_{\alpha\beta}$$

$$+ \frac{1}{4} \sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \sum_{z_1 z_2 z_3 z_4} \sum_{\vec{k} \vec{k}' \vec{k}''} \langle \vec{k} \sigma_1 z_1 \sigma_2 z_2 | \delta \tilde{U}^\dagger | \vec{k}' \sigma_3 z_3 \sigma_4 z_4 \rangle$$

$$\times \sum_{\rho} \phi_{\rho}(\rho) \gamma_{\ell', j'-\sigma}^{m_j'-\sigma}(\Omega_{\vec{p}}) \langle \ell' m_j'-\sigma \pm \sigma | j' m_j' \rangle$$

$$\times \sum_{\rho\sigma\mu\nu} \phi_{\rho}^*(|\vec{k}_\rho + \vec{k}|) \phi_{\sigma}^*(|\vec{k}_\sigma - \vec{k}|) \phi_{\mu}(|\vec{k}_\mu + \vec{k}'|) \phi_{\nu}(|\vec{k}_\nu - \vec{k}'|)$$

$$\times \gamma_{\ell_1, j_1-\sigma_1}^{m_{j_1}-\sigma_1}(\Omega_{\vec{k}_1+\vec{k}}) \gamma_{\ell_2, j_2-\sigma_2}^{m_{j_2}-\sigma_2}(\Omega_{\vec{k}_2-\vec{k}}) \gamma_{\ell_3, j_3-\sigma_3}^{m_{j_3}-\sigma_3}(\Omega_{\vec{k}_3+\vec{k}'}) \gamma_{\ell_4, j_4-\sigma_4}^{m_{j_4}-\sigma_4}(\Omega_{\vec{k}_4-\vec{k}'})$$

$$\times \langle j_1 m_{j_1} | \ell_1 m_{j_1}-\sigma_1 \pm \sigma_1 \rangle \langle j_2 m_{j_2} | \ell_2 m_{j_2}-\sigma_2 \pm \sigma_2 \rangle \langle j_3 m_{j_3} | \ell_3 m_{j_3}-\sigma_3 \pm \sigma_3 \rangle \langle j_4 m_{j_4} | \ell_4 m_{j_4}-\sigma_4 \pm \sigma_4 \rangle$$

$$\times \left[\delta_{\beta\mu} (\delta_{\alpha\mu} \delta_{\sigma\nu} - \delta_{\alpha\nu} \delta_{\sigma\mu}) - \delta_{\beta\sigma} (\delta_{\alpha\mu} \delta_{\rho\nu} - \delta_{\alpha\nu} \delta_{\rho\mu}) \right] \quad (14)$$

(6)

$$= \Phi_\alpha(\rho) Y_{\ell}^{m_j - \sigma}(\Omega_{\vec{\rho}}) \langle \ell m_j - \sigma \pm \sigma | j m_j \rangle$$

$$+ \frac{1}{4} \sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \sum_{\tau_1 \tau_2 \tau_3 \tau_4} \sum_{\vec{k} \vec{k}' \vec{k}''} \langle \vec{k} \sigma_1 \tau_1 \sigma_2 \tau_2 | \delta \tilde{U}^+ | \vec{k}' \sigma_3 \tau_3 \sigma_4 \tau_4 \rangle$$

$$\times \left[\sum_{\beta \sigma} \Phi_\beta(\rho) Y_{\ell'}^{m_j' - \sigma}(\Omega_{\vec{\rho}}) \langle \ell' m_j' - \sigma \pm \sigma | j' m_j' \rangle \right.$$

$$\times \Phi_\beta^*(|\vec{k} + \vec{k}'|) \Phi_\sigma^*(|\vec{k} - \vec{k}'|) \Phi_\alpha(|\vec{k} + \vec{k}''|) \Phi_\sigma(|\vec{k} - \vec{k}''|)$$

$$\times Y_{\ell'}^{m_j' - \sigma_1}(\Omega_{\vec{k} + \vec{k}'}) Y_{\ell_2}^{m_{j_2} - \sigma_2}(\Omega_{\vec{k} - \vec{k}'}) Y_{\ell}^{m_j - \sigma_3}(\Omega_{\vec{k} + \vec{k}''}) Y_{\ell_2}^{m_{j_2} - \sigma_4}(\Omega_{\vec{k} - \vec{k}''})$$

$$\times \langle j' m_j' | \ell' m_j' - \sigma_1 \pm \sigma_1 \rangle \langle j_2 m_{j_2} | \ell_2 m_{j_2} - \sigma_2 \pm \sigma_2 \rangle \langle \ell m_j - \sigma_3 \pm \sigma_3 | j m_j \rangle$$

$$\times \langle \ell_2 m_{j_2} - \sigma_4 \pm \sigma_4 | j_2 m_{j_2} \rangle - 3 \text{ other terms} \quad (15)$$

* should $\delta_{\beta\beta} \Rightarrow m_{\ell'} = m_{\ell_1}$?

(s.p.)

$$\text{Let } \sigma, j_1, m_{j_1}, \ell_1 \rightarrow \gamma, j'', m_{j''}, \ell''$$

Then Eq. (15) reads

$$= \Phi_\alpha(\rho) Y_{\ell}^{m_j - \sigma}(\Omega_{\vec{\rho}}) \langle \ell m_j - \sigma \pm \sigma | j m_j \rangle$$

$$+ \frac{1}{4} \sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \sum_{\tau_1 \tau_2 \tau_3 \tau_4} \sum_{\vec{k} \vec{k}' \vec{k}''} \langle \vec{k} \sigma_1 \tau_1 \sigma_2 \tau_2 | \delta \tilde{U}^+ | \vec{k}' \sigma_3 \tau_3 \sigma_4 \tau_4 \rangle$$

$$\times \sum_{\beta \gamma} \left[\Phi_\beta(\rho) \Phi_\beta^*(|\vec{k} + \vec{k}'|) \Phi_\gamma^*(|\vec{k} - \vec{k}'|) \Phi_\gamma(|\vec{k} + \vec{k}''|) \Phi_\alpha(|\vec{k} - \vec{k}''|) \right.$$

$$\times Y_{\ell'}^{m_j' - \sigma}(\Omega_{\vec{p}}) \langle \ell' m_j' - \sigma \pm \sigma | j' m_j' \rangle Y_{\ell'}^{m_j' - \sigma_1^*}(\Omega_{\vec{k}_2 + \vec{u}}) \langle \ell' m_j' | \ell' m_j' - \sigma_1 \pm \sigma_1 \rangle \quad (7)$$

$$\times Y_{\ell''}^{m_j'' - \sigma_2^*}(\Omega_{\vec{k}_2 + \vec{u}}) \langle j'' m_j'' | \ell'' m_j'' - \sigma_2 \pm \sigma_2 \rangle Y_{\ell''}^{m_j'' - \sigma_4}(\Omega_{\vec{k}_2 + \vec{u}}) \langle \ell'' m_j'' - \sigma_4 \pm \sigma_4 | j'' m_j'' \rangle$$

$$\times Y_{\ell}^{m_j - \sigma_3}(\Omega_{\vec{k}_1 + \vec{u}}) \langle \ell m_j - \sigma_3 \pm \sigma_3 | j m_j \rangle - 3 \text{ other terms} \quad (16)$$

$$[\Phi] = f m^{3/2} \quad [S U^+] = f m^3 \quad \left[\sum_{\vec{k}, \vec{u}, \vec{u}'} \right] = f m^{-9}$$

$$\Rightarrow \left[\sum_{\vec{k}, \vec{u}, \vec{u}'} \Phi \Phi^* \Phi^* \Phi \Phi S U^+ \right] = f m^{3/2} \quad \checkmark$$

Questions :

i) How do we reduce $Y_{\ell}^{m_{\ell}}$ dependencies?

$Y_{\ell}^{m_{\ell}}$ have different Ω dependencies and ℓ, m_{ℓ} dependencies.

ii) Does the $\sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4}$ simplify at all?

iii) First term is simple :

$$S_{\alpha} = \frac{1}{j+1} \sum_{m_j} \int d^3 p \left| \Phi_{\alpha}(p) Y_{\ell}^{m_j - \sigma}(\Omega_{\vec{p}}) \langle \ell m_j - \sigma \pm \sigma | j m_j \rangle \right|^2$$

$$\sum_{m_j} \int d\Omega_{\vec{r}} \left| \Phi_{\alpha}(\rho) Y_{\ell}^{m_j - \sigma}(\Omega_{\vec{r}}) \langle \ell m_j - \sigma \frac{1}{2} \sigma | j m_j \rangle \right|^2$$

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$$= (2j+1) \left| \Phi_{\alpha}(\rho) \right|^2$$

$$\Rightarrow S_{\alpha} = \frac{1}{4j+1} (2j+1) \int d\rho \rho^2 \left| \Phi_{\alpha}(\rho) \right|^2$$

$$= 1 \quad \checkmark$$