multi-reference equation of motion

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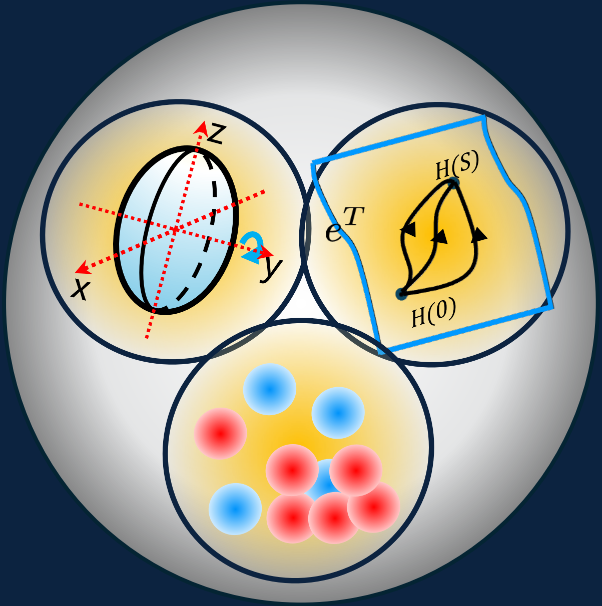

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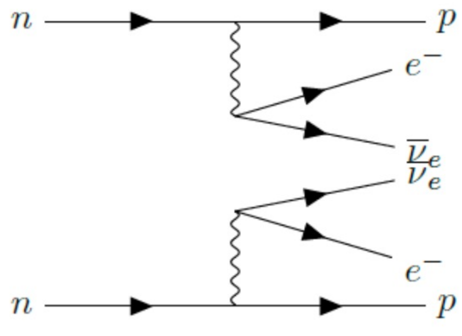
$2\nu\beta\beta$ decay nuclear matrix element

The half-life of $2\nu\beta\beta$ depends on the nuclear matrix elements

$$\left(T_{1/2}^{2\nu}\right)^{-1} = G^{2\nu} g_A^4 \left(M^{2\nu}\right)^2,$$

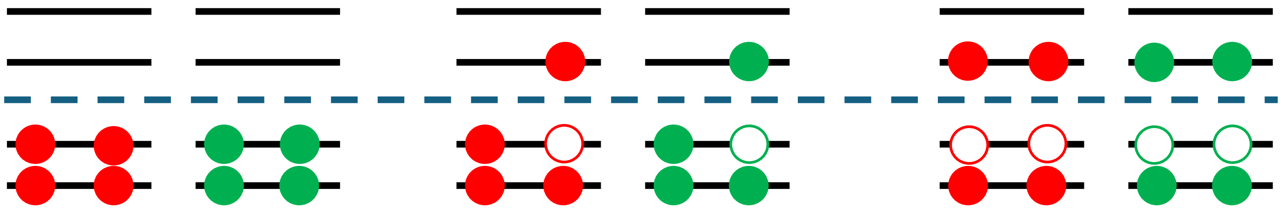
$$M^{2\nu} = \sum_k \frac{\langle 0_f^+ || \sum_a \tau_a^- \boldsymbol{\sigma}_a || 1_k^+ \rangle \langle 1_k^+ || \sum_b \tau_b^- \boldsymbol{\sigma}_b || 0_i^+ \rangle}{(E_k - (E_i + E_f)/2)/m_e}$$



Need to compute the ground state of initial and final nuclei, as well as the all-excited $1^+(0^+)$ state of intermediate nuclei for the Gamow-Teller (Fermi) operator

Challenges to get accurate high-lying states of the intermediate nuclei.

How do we compute the states of nuclei?



- all possible configurations
- Huge, sparse Matrix
- Diagonalization to get energy and wavefunction

$$H \begin{pmatrix} |\Psi_{\rm ex}\rangle \\ \cdots \\ |\Psi_0\rangle \end{pmatrix} = E \begin{pmatrix} |\Psi_{\rm ex}\rangle \\ \cdots \\ |\Psi_0\rangle \end{pmatrix}$$

$10^8 \approx$ 500 MB in memory for one vector

10^{12} is almost the limit of classic computer

dim $\approx N^A$ (exponential scale)

$\approx 2000^A$

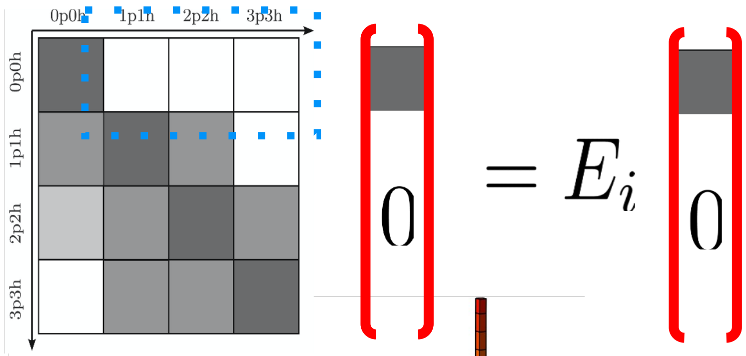
Ab-initio nuclear structure calculation with polynomial scaling(Coupled Cluster, IM-SRG,..)

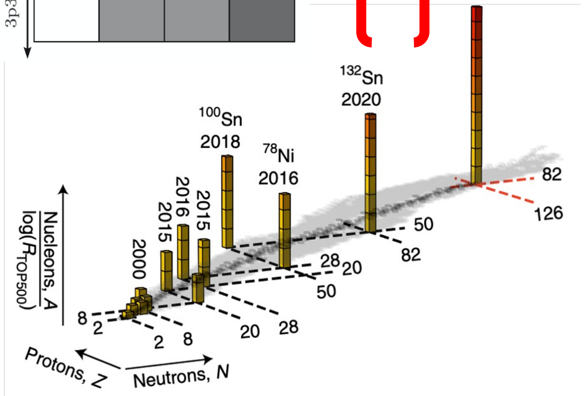
$$\langle \Psi_0 | e^{-T} H e^T | \Psi_0 \rangle = E$$

$$\langle \Psi_{ij\ldots}^{ab\ldots} | e^{-T} H e^T | \Psi_0 \rangle = 0$$

$$\hat{T} = \sum_i T_i$$ Excitation operators

$$\hat{T}_1 = \sum_{ia} t_i \alpha_a^\dagger \alpha_i, \quad \hat{T}_2 = \frac{1}{2} \sum_{i<j, a<b} t_{ij}^{ab} \alpha_a^\dagger \alpha_b^\dagger \alpha_i \alpha_j$$

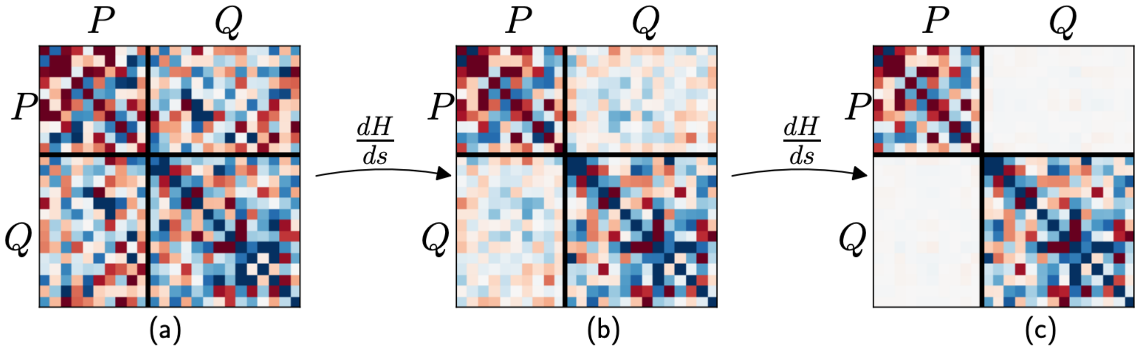




Hu, *et al*, Nature physics, **18**, 1196. (2022)

Similarity transformation, decoupled the ground state, Polynomial scale

How we compute open shell nuclei (VS-IMSRG, CC)



Annu. Rev. Nucl. Part. Sci. 69:307

$$\eta^{\mathrm{Wh}}(s) \equiv \frac{H^{od}(s)}{\Delta(s)}.$$

$$|\Psi\rangle = C_0(1 + \frac{C_i^a}{C_0} a^\dagger i + \frac{C_{ij}^{ab}}{C_0} a^\dagger b^\dagger ij + \cdots)|\Psi_0\rangle = P|\Psi_0\rangle + Q|\Psi_0\rangle \propto e^S|0\rangle$$

- The true state should be dominated by the reference, otherwise $(C_0 = 0)$ T , S or Ω may diverge for operators with any rank.
- Low-lying states, the quality and accuracy depends on the shell gap
- High energy states: multi-shell effective interaction, vanished energy denominator, intruder states, etc.

A long-term effort to tackle intruder states

A shell-model description of 0^+ intruder states in even-even nuclei

K. Heyde, J. Jolie [1], J. Moreau [2], J. Ryckebusch [1], M. Waroquier [3], P. Van Duppen, M. Huyse, J.L. Wood Show more

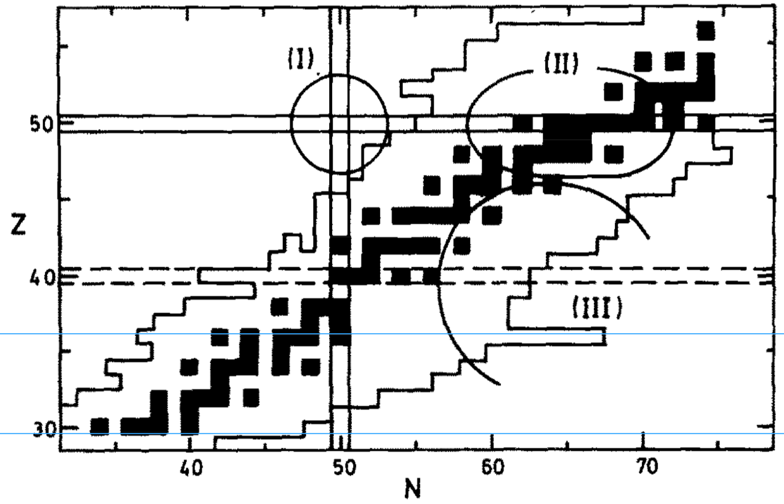


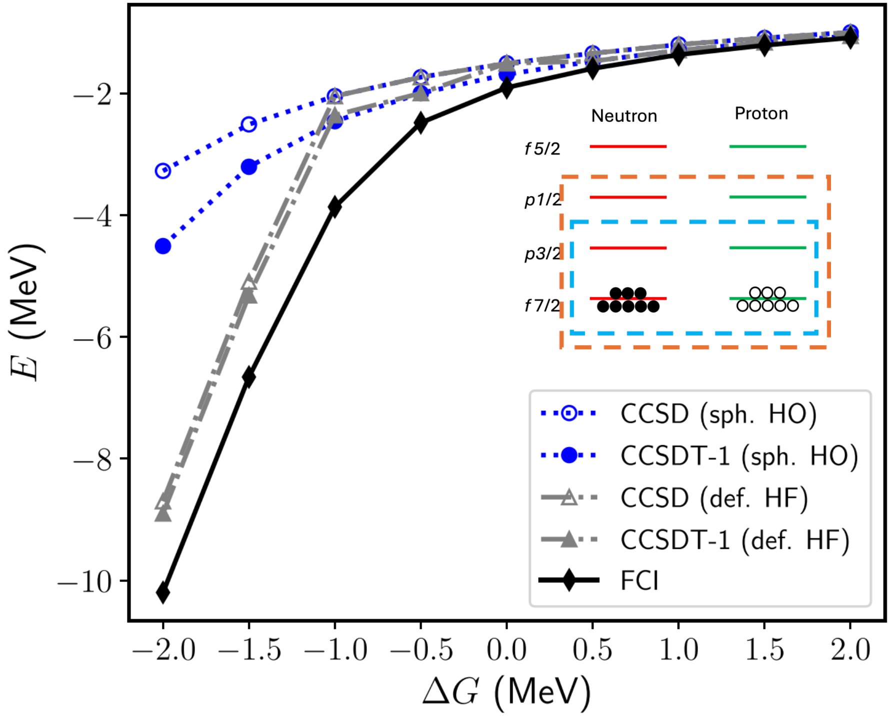
Fig. 1. Schematic division of nuclei in the $Z \simeq 40$, 50 and $50 \leqslant N \leqslant 82$ mass table into three major regions, i.e. (I) region near doubly-closed shells; (II) region of possible intruder states; (III) region of strongly deformed nuclei.

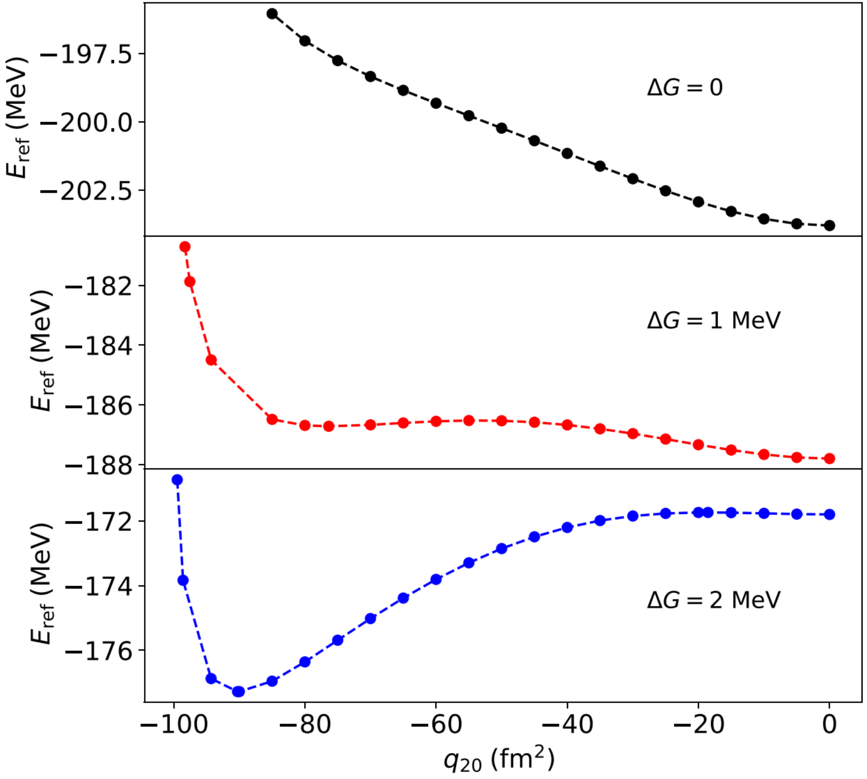
$$\frac{\langle \Psi_\mu | Q | \Psi_\mu \rangle}{\langle \Psi_\mu | \Psi_\mu \rangle} = \frac{\rho_Q}{1+\rho_Q} \lesssim \frac{1}{2}$$

K. Suzuki , Shyh Yuan Lee. *PTP*. 64, 2091(1980)

P space components should be dominant in the wavefunction

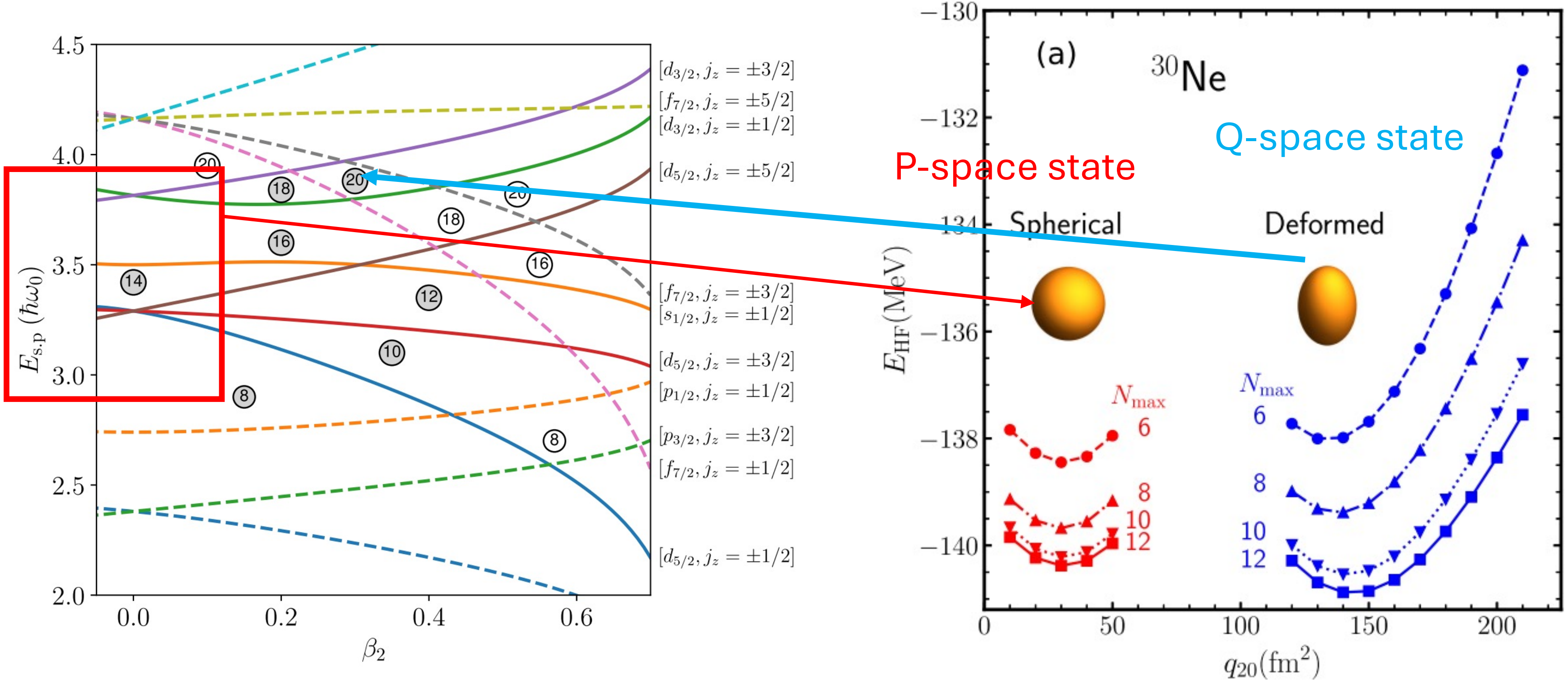
Example: vanished shell gap(quasi degenerate)





Strong entanglement, spontaneously rotational symmetry breaking, deformation.

Deformation emerge as vanished shell gap



intruder state, level crossing, deformation, cluster structure…

Equation of Motion method,

The standard problem: $$H|\mu\rangle = E_\mu|\mu\rangle$$

We focus on specified excitation mode the excited state on top of a reference state

$$|\mu\rangle = Q^\dagger_\mu|0\rangle \qquad Q_\mu|0\rangle = 0 \qquad Q^\dagger_\mu = \sum_\alpha X^\mu_\alpha \eta^\dagger_\alpha$$

EOM Secular equation:

$$\sum_\beta \langle 0|[\eta_\alpha,[H,\eta^\dagger_\beta]]|0\rangle X^\mu_\beta = \delta E_\mu \sum_\beta \langle 0|[\eta_\alpha,\eta^\dagger_\beta]|0\rangle X^\mu_\beta$$

Systematically truncated to fit available computational power and the physics of interest

D.J. Rowe. Rev. Mod. Phys. **40**, 153

Equation of motion coupled cluster

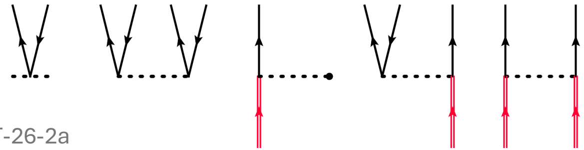
Equation of motion method to get excited states, particle attached, charge exchange

$$(\bar{H}\hat{R}_{\mu}^{(A\pm2)})_C|\Phi_0\rangle = \omega_\mu \hat{R}_{\mu}^{(A\pm2)}|\Phi_0\rangle$$

G. R. Jansen, *et al*, Phys. Rev. C 83, 054306

Operator	Expression
$\hat{R}^{A+2}_{2p-0h}$	$\frac{1}{2}\sum_{ab} r^{ab} a^\dagger_a a^\dagger_b$
$\hat{R}^{A+2}_{3p-1h}$	$\frac{1}{2}\sum_{ab} r^{ab} a^\dagger_a a^\dagger_b + \frac{1}{6}\sum_{abci} r^{abc}_i a^\dagger_a a^\dagger_b a^\dagger_c a_i$
$\hat{R}^{A-2}_{0p-2h}$	$\frac{1}{2}\sum_{ij} r_{ij} a_j a_i$
$\hat{R}^{A-2}_{1p-3h}$	$\frac{1}{2}\sum_{ij} r_{ij} a_j a_i + \frac{1}{6}\sum_{aijk} r^a_{ijk} a^\dagger_a a_k a_j a_i$

Method	**Reference State** $\|0\rangle$	**Generator** $O^\dagger_\nu$
HF	$\|\mathrm{HF}\rangle$	$a^\dagger_m a_i$
TDA	$\|\mathrm{HF}\rangle$	$\sum_{mi} X^\nu_{mi} a^\dagger_m a_i$
RPA	$\|\mathrm{RPA}\rangle$	$\sum_{mi}\left(X^\nu_{mi} a^\dagger_m a_i - Y^\nu_{mi} a^\dagger_i a_m\right)$
HFB	$\|\mathrm{HFB}\rangle$	$\alpha^\dagger_k \alpha^\dagger_{k'}$
QRPA	$\|\mathrm{QRPA}\rangle$	$\sum_{k<k'}\left(X^\nu_{kk'} \alpha^\dagger_k \alpha^\dagger_{k'} - Y^\nu_{kk'} \alpha_{k'} \alpha_k\right)$
MR-EOM	$\|\mathrm{sm\quad state}\rangle$	


(a) (b) (c) (d) (e)

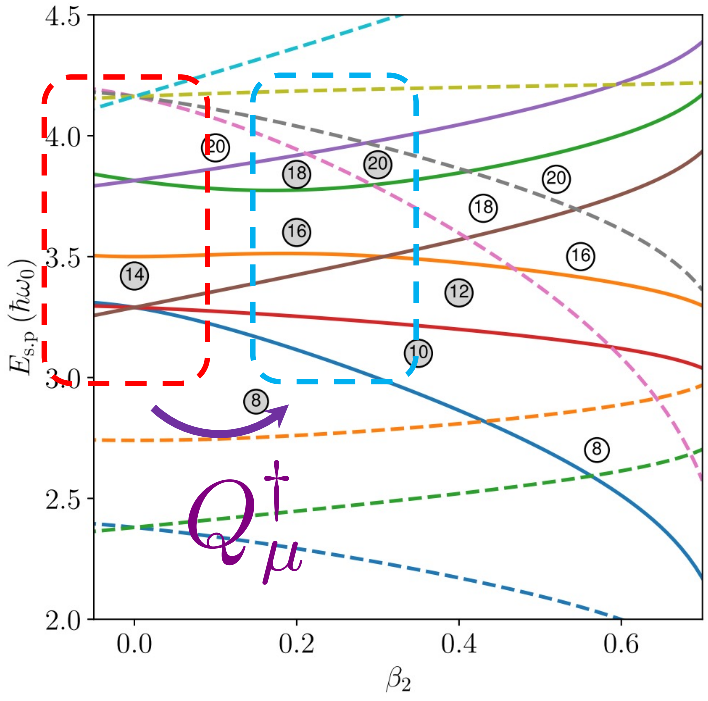
Equation of Motion method, excitations on top of a “good” reference

The shell model state as a reference state

$$|\Psi_0\rangle = e^{\Omega}|\nu^n\rangle$$

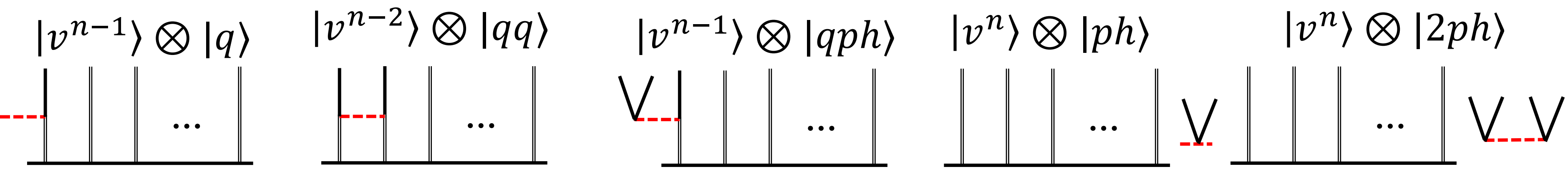
An intruder state could be a collective 1-particle-1-hole, 2-particle-2-hole excitation on top of the shell model state

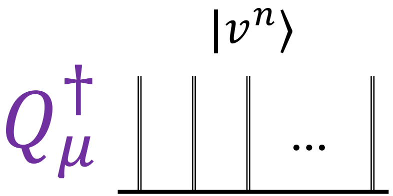
$$|\Psi^{\mu}\rangle = Q_{\mu}^{\dagger}|\Psi_0\rangle$$



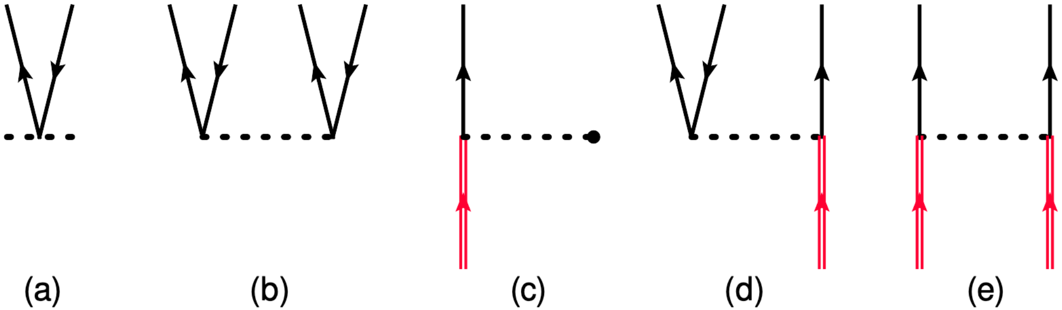
$Q_{\mu}^{\dagger}$ has a systematically hierarchy of order-by-order truncations

Equation of motion on top of a shell model state





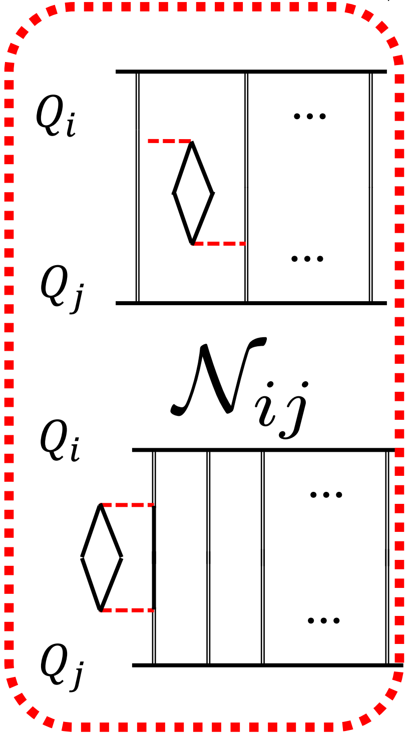
$$Q_\mu^\dagger|\Phi_0\rangle = 0$$

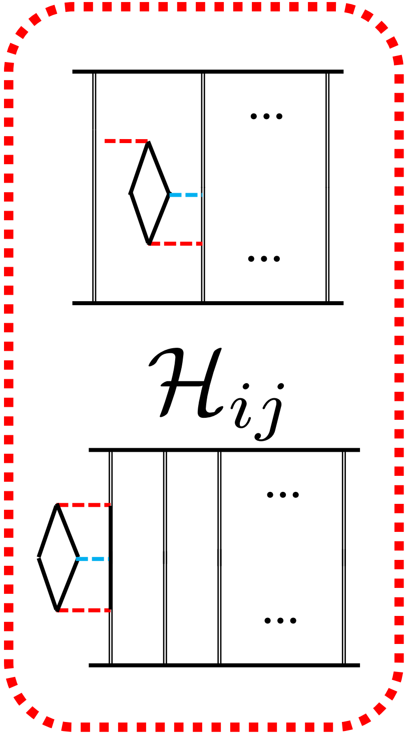


- Pick a reference state from the model space
- Generate excited states (automatically orthogonalized to all state inside the model space)
- Solve the equation of motion in the Fock space (two- and three-body operators)

Equation of motion on top of a shell model state

$$\sum_\beta \langle 0|[\eta_\alpha,[H,\eta_\beta^\dagger]]|0\rangle X_\beta^\mu = \delta E_\mu \sum_\beta \langle 0|[\eta_\alpha,\eta_\beta^\dagger]|0\rangle X_\beta^\mu$$





- The Norm and Hamiltonian matrix (kernels) come as one-, two and three-body operators inside the model space. Its matrix elements are computed as expectation of these operators respect to the reference (shell model state).

$$\mathcal{H}_{ij} = \mathrm{Tr}[(Q_i^\dagger Q_j)_c^{(k)}\rho^{(k)}]$$

- Order-by-order approximation on the truncation of Q_μ.
- The EOM is solved in the Fock space, suppose to work for any nuclei for a given model space

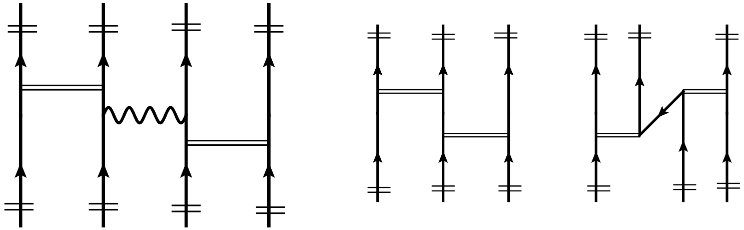
How to solve the EOM

- Lanczos or Arnoldi algorithm

$$(HQ_i)_c|0\rangle = \beta_{i+1}Q_{i+1}|0\rangle + \alpha_i Q_i|0\rangle + \beta_i Q_{i-1}|0\rangle$$

$$\alpha_i = [Q_i, [H, Q_j]]$$ Up to 4-body

$$\beta_i = [\tilde{Q}_i, \tilde{Q}_i^\dagger]$$ Up to 3-body

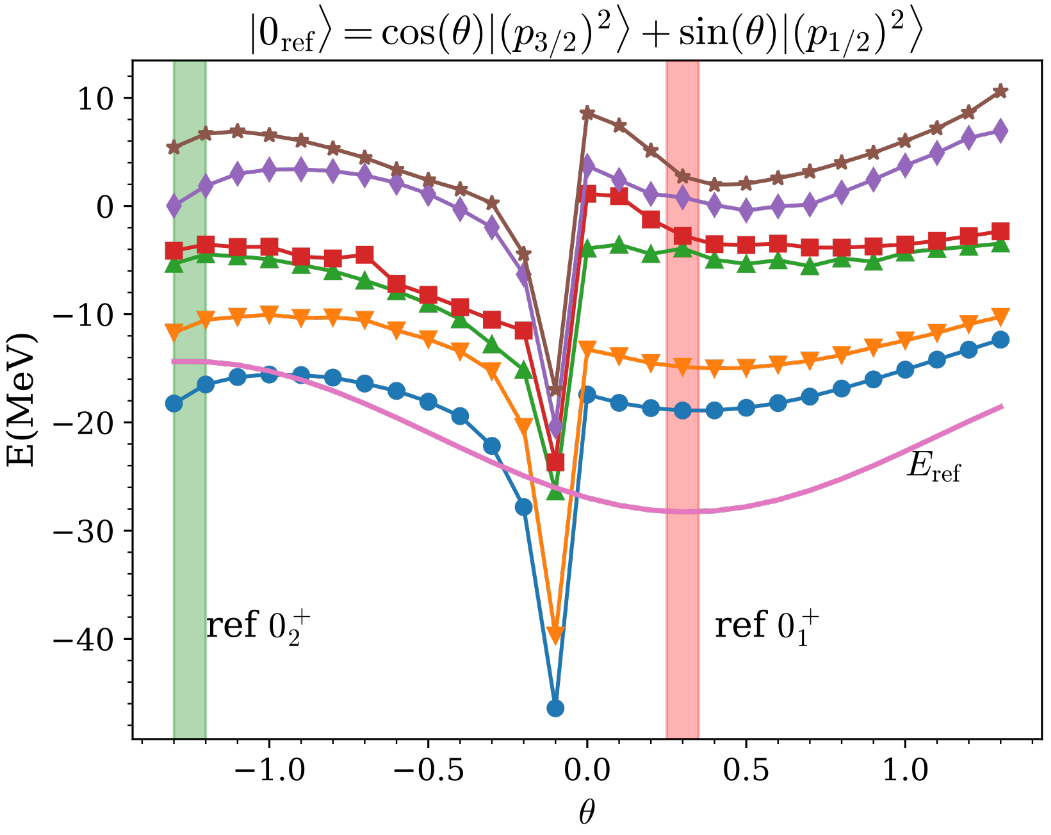


Problem:

1. truncation error leads to failure of Lanczos algorithm, include 3-body intermediate in Arnoldi.

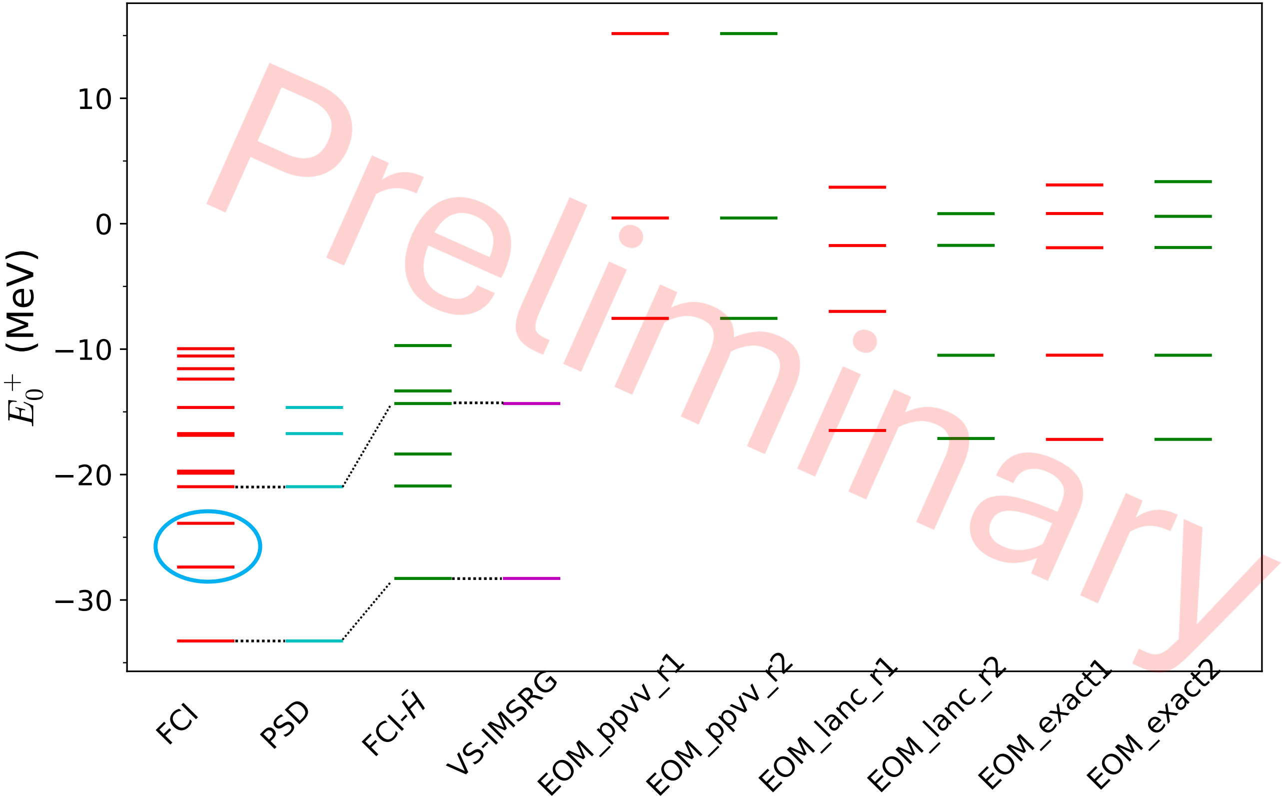
2. Overcomplete basis, $\sum_k ||Q_i^k||^2$ become numerical huge though is one $\langle 0|[\tilde{Q}_i, \tilde{Q}_i^\dagger]|0\rangle$, spurious states. SVD on the Norm matrix to remove redundant degree of freedom

Picking accurate reference state



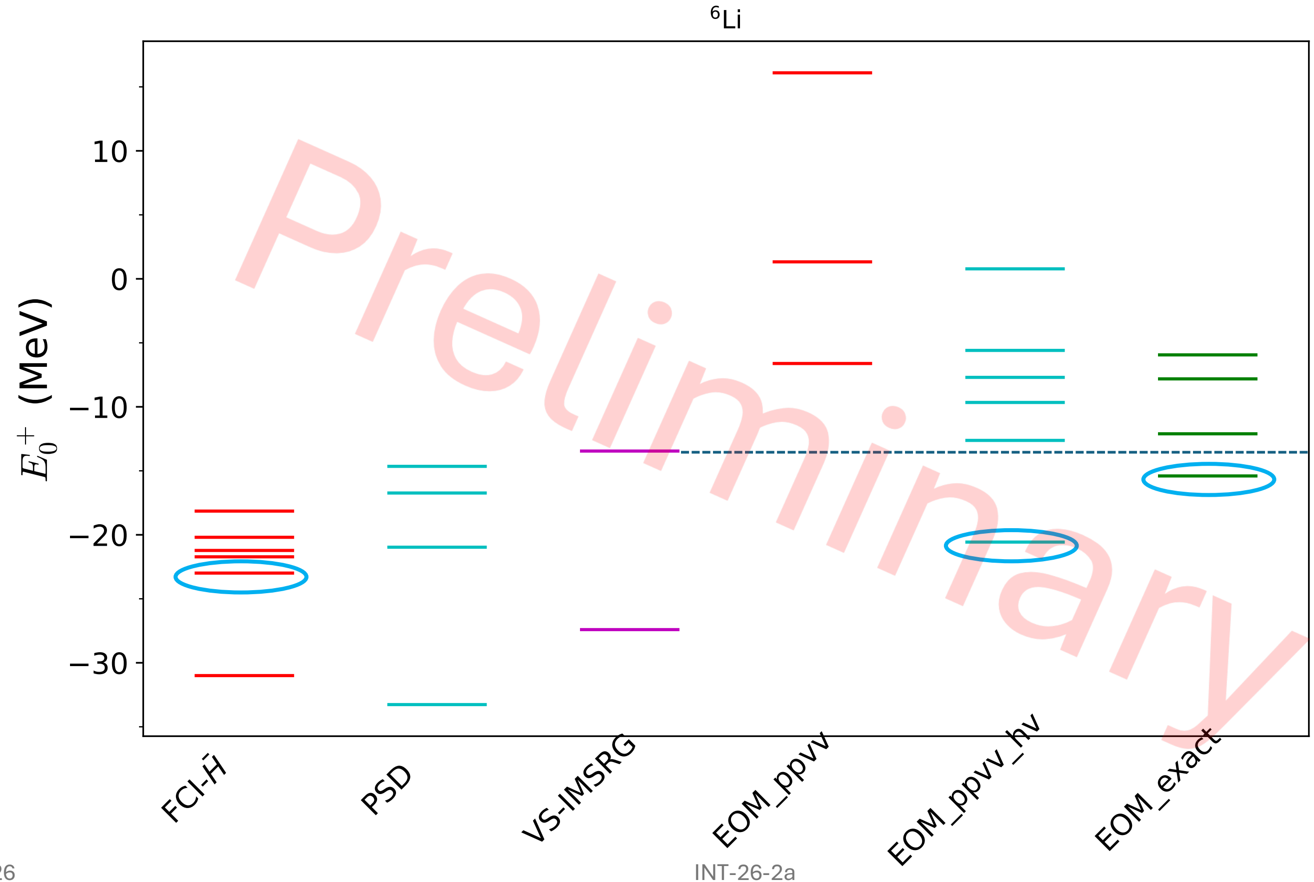
For Simple system: Based on two different valence states of ^{6}He, we roughly get the same spectrum from EOM calculation.

0^+ states of ^{6}He, N_{max}=2



The shell-model-EOM captured the intruder states, as well as other high lying states.

1^+ states of ^{6}Li, N_{max}=2



Summary and outlook

- An equation of motion method on top of a shell model state (multiple reference).
- Excitations defined in Fock space as two body operators.
- The norm (overlap) and Hamiltonian kernel is computed as expectation of operators on shell model wavefunction,
- Applied to two valence particle system (He, Li), scalar excitation ($0^+ \to 0^+$, $1^+ \to 1^+$)
- Working on generate tensor excitations ($0^+ \to 1^+$)

Thank you!