26th Sep. 2011

Many-body perturbation approach to effective interaction for the shell model

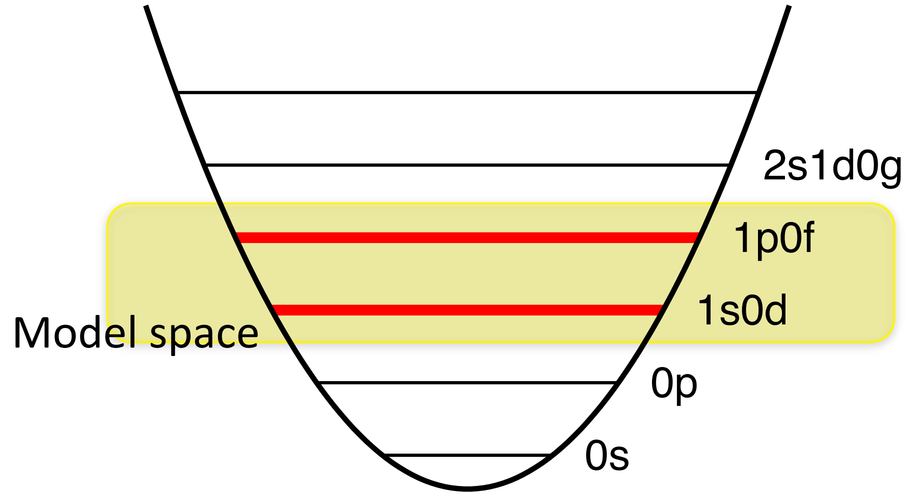
Naofumi Tsunoda
Univ. Tokyo

collaborators:

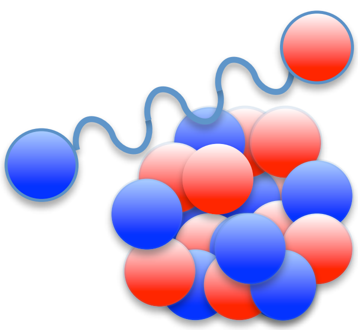
Kazuo Takayanagi (Sofia. U)
Morten Hjorth-Jensen (Oslo. U)
Takaharu Otsuka (Tokyo. U)

Motivation

- Nuclear shell model
  - Effective interaction defined in the model space
  - Single particle energies



Nuclear force in nuclear medium

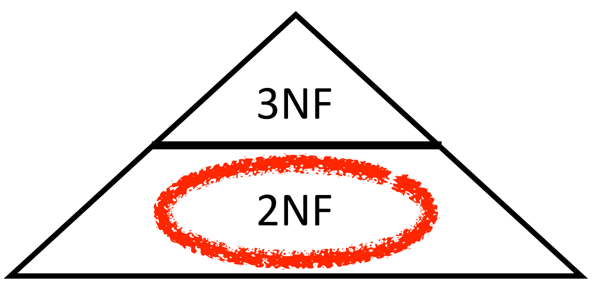


emprically or microscopically derived

→ Nuclear properties

Motivation

- Obtain effective interaction for the shell model for **multi-shell** calculation
  - Many-body perturbation theory to obtain effective interaction is, usually, only capable in single major shell.
  - *Fully microscopic* description of the nuclei far from stability
    - Currently only *phenomenological* effective interaction is used for those calculations
  - *psd*-shell nuclei
    - Neutron halo, etc.
  - *sdpf*-shell nuclei
    - Island of inversion, etc.



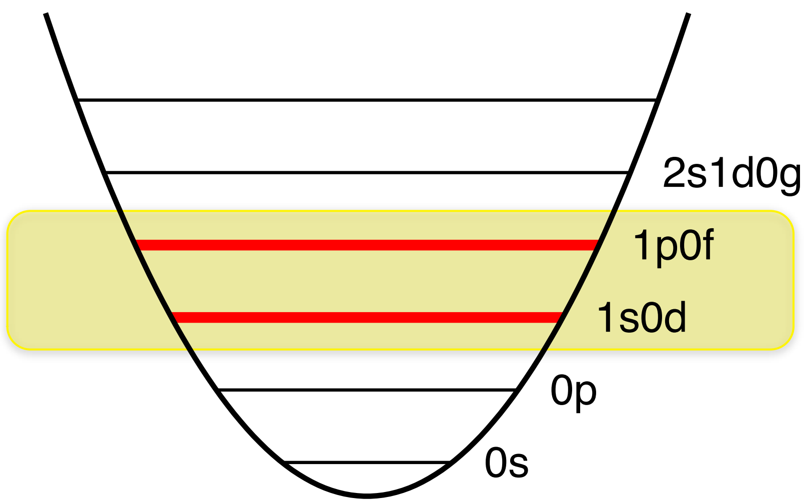


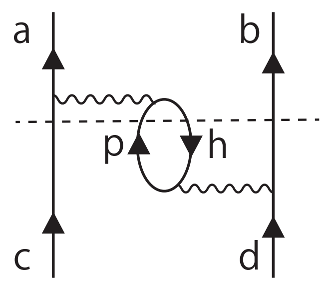
Table of Contents

Effective interaction for the shell model

	Empirical matrix element	MBPT
Starting from NN interaction	△	◎ (with soft interaction)
Agreement with Experiments	◎	○
Multi-shell calculation	◎	△

- Many-body perturbation theory (MBPT) starting from soft interaction
  - Vlowk, G-matrix, Vsrg
  - Limited to the case of unperturbed model space is **degenerated**

Example: 3p1h diagram



$$\frac{V_{cpah}V_{hdpb}}{\epsilon_d - \epsilon_b - \epsilon_p + \epsilon_h}$$

If the model space is not degenerated…

- **Divergent** or **nearly divergent**
- *Strong **non-Hermiticity***

New method overcome this limitation

3. Review of MBPT (Kuo-Krenciglowa method)

Formal theory

Definitions and setups

$$H|\Psi_\lambda\rangle = E_\lambda|\Psi_\lambda\rangle \qquad P^2 = P, \quad P + Q = 1 \qquad \lambda = 1, 2, \cdots, d, \cdots, n$$

$$P|\Psi_i\rangle = |\Phi_i\rangle \qquad \omega|\Phi_i\rangle = Q|\Psi_i\rangle \qquad Q\omega P = \omega \qquad i = 1, 2, \cdots, d$$

$$\mathcal{H} = e^{-\omega} H e^{\omega}$$

(Similarity transf. : yields the **same** eigenvalues as original Hamiltonian H)

Decoupling equation

$$\begin{pmatrix} P\mathcal{H}P & P\mathcal{H}Q \\ Q\mathcal{H}P & Q\mathcal{H}Q \end{pmatrix}$$

$$0 = Q\mathcal{H}P = QVP - \omega PHP + QHQ\omega - \omega PVQ\omega$$

Effective Hamiltonian

$$H_{\mathrm{eff}} = P\mathcal{H}P \qquad H_{\mathrm{eff}}|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$V_{\mathrm{eff}} = PVP + PVQ\omega, \quad H_{\mathrm{eff}} = PHP + PVQ\omega$$

Veff: Effective interaction defined in purely in P-space

Problem: How can we obtain ω which fulfill the decoupling equation?

Kuo-Krenciglowa (KK) method

Krenciglowa and Kuo Nucl.Phys.A **235** 171 (1974)

Iterative solution of decoupling equation

$$0 = Q\mathcal{H}P = QVP - \omega PHP + QHQ\omega - \omega PVQ\omega$$

$PH_0P = \epsilon_0$ (Degenerate model space is assumed)

$$(\epsilon_0 - QHQ)\omega = QVP - \omega PVP - \omega PVQ\omega$$

$$\omega = \frac{1}{\epsilon_0 - QHQ} QVP - \frac{1}{\epsilon_0 - QHQ}\omega V_{\mathrm{eff}}$$

$$V_{\mathrm{eff}} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0)\{V_{\mathrm{eff}}\}^k$$

Solve this equation iteratively

Q-box $\hat{Q}(\epsilon) = PVP + PVQ\dfrac{1}{\epsilon - QHQ}QVP$ $\quad \hat{Q}_k(\epsilon_0) = \dfrac{1}{k!}\{\dfrac{\mathrm{d}^k\hat{Q}}{\mathrm{d}\epsilon}\}_{\epsilon=\epsilon_0}$

4. EKK method

Extended KK (EKK) method

Takayanagi Nucl.Phys.A **852(1)** 61 (2011)

Decoupling equation

$$0 = Q\mathcal{H}P = QVP - \omega PHP + QHQ\omega - \omega PVQ\omega$$

$$(\boxed{E} - QHQ)\omega = QVP - \omega P\tilde{H}P - \omega PVQ\omega$$

arbitrary constant energy parameter

$$\omega = \frac{1}{E-QHQ}QVP - \frac{1}{E-QHQ}\omega\tilde{H}_{\mathrm{eff}}$$

$$\tilde{H}_{\mathrm{eff}} = \tilde{H}_{\mathrm{BH}}(E) + \sum_{k=1}^{\infty}\hat{Q}_k(E)\{\tilde{H}_{\mathrm{eff}}\}^k$$

$$\tilde{H} = H - E \qquad H_{\mathrm{BH}}(\epsilon) = PHP + PVQ\frac{1}{\epsilon - QHQ}QVP$$

- No need of degenerate model space
- E is an ***arbitrary*** constant energy parameter
- It works excellently in 4 dimensional model Hamiltonian! (Ref.)

Time dependent perturbation theory

$$Q' = Q - PVP$$ (start from second order)

$$V_{\mathrm{eff}} = \hat{Q}(\epsilon_0) - \hat{Q}'(\epsilon_0)\int \hat{Q}(\epsilon_0) + \hat{Q}'(\epsilon_0)\int \hat{Q}(\epsilon_0)\int \hat{Q}(\epsilon_0) + \cdots$$

$$V_{\mathrm{eff}} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0)\{V_{\mathrm{eff}}\}^k$$

- Folded diagrams can be calculated by **energy derivatives**
  - *Only if* the unperturbed Hamiltonian is *degenerate* in P-space
- One only need the value of Q-box and its derivatives at a single point
- Numerical calculations are based on this time dependent perturbation theory because we need diagramatic description of Q-box

EKK from the perspective of TDPT

$$H = \begin{pmatrix} PHP & PHQ \\ QHP & QHQ \end{pmatrix} = \boxed{\begin{pmatrix} PH_0P & 0 \\ 0 & QH_0Q \end{pmatrix} + \begin{pmatrix} PVP & PVQ \\ QVP & QVQ \end{pmatrix}} \quad \text{I.KK}$$

$$= \boxed{\begin{pmatrix} E & 0 \\ 0 & QH_0Q \end{pmatrix} + \begin{pmatrix} P\tilde{H}P & PVQ \\ QVP & QVQ \end{pmatrix}} \quad \text{II.EKK}$$

$$\rightarrow \quad H_{\text{eff}} = \underline{\hat{Q}}(\epsilon_0) - \underline{\hat{Q}'}(\epsilon_0) \int \underline{\hat{Q}}(\epsilon_0) + \underline{\hat{Q}'}(\epsilon_0) \int \underline{\hat{Q}}(\epsilon_0) \int \underline{\hat{Q}}(\epsilon_0) + \cdots$$

$$\underline{\hat{Q}}(E) = P\tilde{H}P + PVQ\frac{1}{E - QHQ}QVP = \tilde{H}_{\text{BH}}(E)$$

- Change the definition of H_0 and V
  - ***Only*** PHP part is changed
  - Folded diagram theory can be used ***in the same way*** except for changing the point where Q-box is evaluated

Evaluation of Q-box by diagrams

$$\langle \Psi_i | V_{\rm eff} | \Psi_j \rangle = \langle \Psi_i | H_{1,I}(0) U_{QV}(0,-\infty) | \Psi_j \rangle$$

KK method

Unperturbed Hamiltonian

$$H_0 = \sum_i \epsilon_i a_i^\dagger a_i$$

$$a_{i,I}^\dagger(t) = e^{i\epsilon_i t} a_i^\dagger$$
$$a_{i,I}(t) = e^{-i\epsilon_i t} a_i$$

EKK method

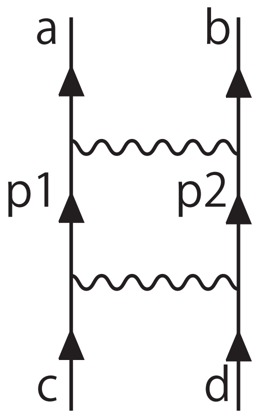
Unperturbed Hamiltonian

$$H_0 = PEP + Q\sum_i (\epsilon_i a_i^\dagger a_i) Q$$

$$P = \sum_{i=1}^{d} |\Phi_i\rangle\langle\Phi_i| = \sum_{i,j=\mathrm{act.}} a_i^\dagger a_j^\dagger |c\rangle\langle c| a_j a_i, \quad Q = 1 - P$$

$$e^{-iH_0 t} a_i^\dagger a_j^\dagger |c\rangle = e^{-iEt} a_i^\dagger a_j^\dagger |c\rangle$$

$$e^{-iH_0 t} a_i^\dagger a_j^\dagger a_p^\dagger a_h |c\rangle = e^{-i(\epsilon_i+\epsilon_j+\epsilon_p-\epsilon_h)t} a_i^\dagger a_j^\dagger a_p^\dagger a_h |c\rangle$$



$$\langle c | a_b a_a H_1 \int_{-\infty}^{0} \mathrm{d}t_1 H_1(t_1) a_a^\dagger a_b^\dagger |c\rangle$$

t=0 $\rightarrow \langle c | a_b a_a \left(a_a^\dagger a_b^\dagger V_{ab,p_1p_2} a_{p_2} a_{p_1} \right) \int_{-\infty}^{0} \mathrm{d}t_1 \left(e^{iH_0 t_1} a_{p_1}^\dagger a_{p_2}^\dagger V_{p_1p_2,cd} a_d a_c e^{-iH_0 t_1} \right) a_c^\dagger a_d^\dagger |c\rangle$

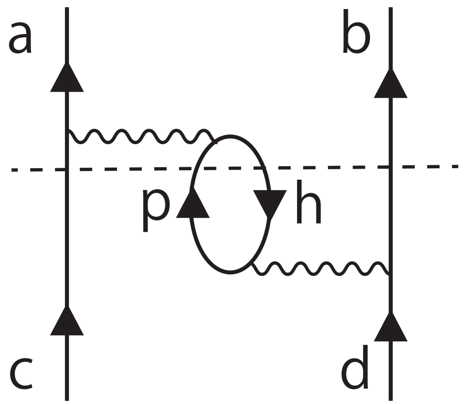
t=t1 $= \langle c | a_b a_a \left(a_a^\dagger a_b^\dagger V_{ab,p_1p_2} a_{p_2} a_{p_1} \right) \int_{-\infty}^{0} \mathrm{d}t_1 \left(e^{iH_0 t_1} a_{p_1}^\dagger a_{p_2}^\dagger V_{p_1p_2,cd} a_d a_c \right) a_c^\dagger a_d^\dagger |c\rangle e^{-iEt_1}$

$$= \frac{V_{ab,p_1p_2} V_{p_1p_2,cd}}{E - \epsilon_{p_1} - \epsilon_{p_2}}$$

Evaluation of Q-box

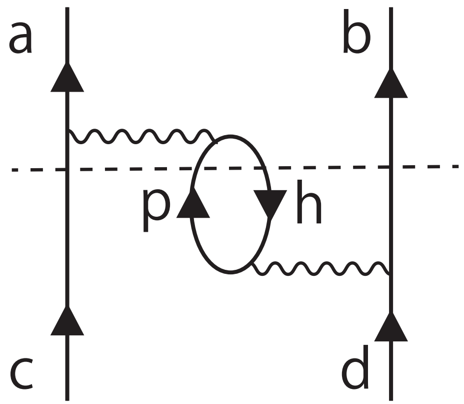
Example: core-polarization diagram

KK method



$$\frac{V_{cpah}V_{hdpb}}{\epsilon_d - \epsilon_b - \epsilon_p + \epsilon_h}$$

EKK method



$$\frac{V_{cpah}V_{hdpb}}{E - (\epsilon_c + \epsilon_b + \epsilon_p - \epsilon_h)}$$

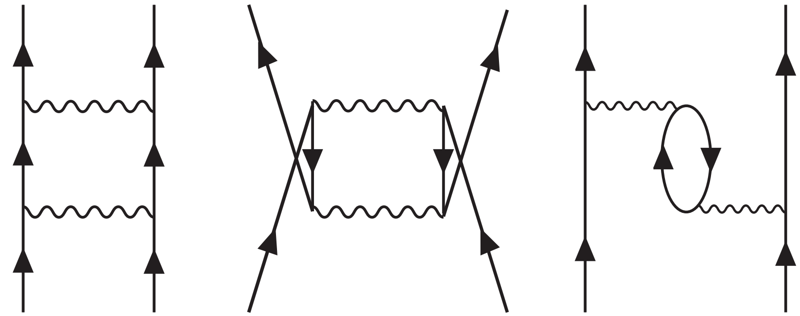
5. Numerical results

Setup of the calculation

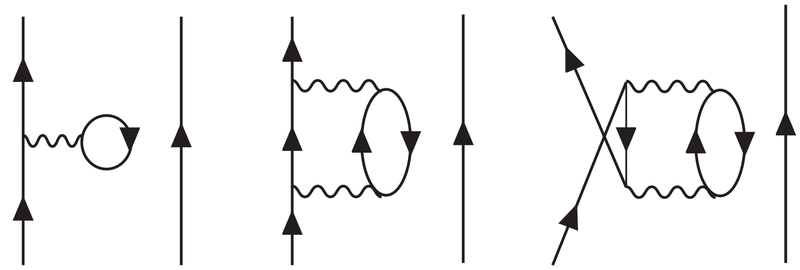
- Q-box is calculated up to second or third order in interaction
- Whole space is taken as 13 major shells
- HF basis (Strictly speaking, only feasible in EKK method and not in KK method)

<u>Examples of the diagrams included in Q-box</u>

Pure two-body contribution



One-body to two-body contribution



E-independence of the EKK method

$$\tilde{H}_{\mathrm{eff}} = \tilde{H}_{\mathrm{BH}}(E) + \sum_{k=1}^{\infty} \hat{Q}_k(E)\{\tilde{H}_{\mathrm{eff}}\}^k$$

$$\tilde{H} = H - E$$

The final result should not depend on the parameter E if there is ***no*** *approximation* in the calculation of Q-box

★ E dependence is a good measure to know the accuracy of the approximation

★ Q-box itself depends on E

★ Folded diagrams restore the E independence

★Ground state energy of O18 and its excitation level will be discussed

★Neutron-neutron interaction is calculated as a test calculation

*V*eff for *sd*-shell

E-independence of the EKK method

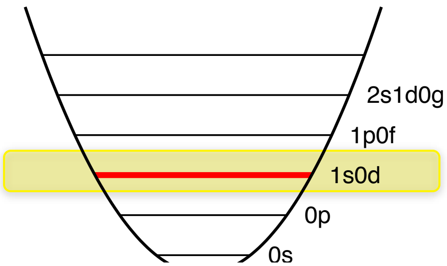
O18 with respect to O16

Empirical sp energies from USD

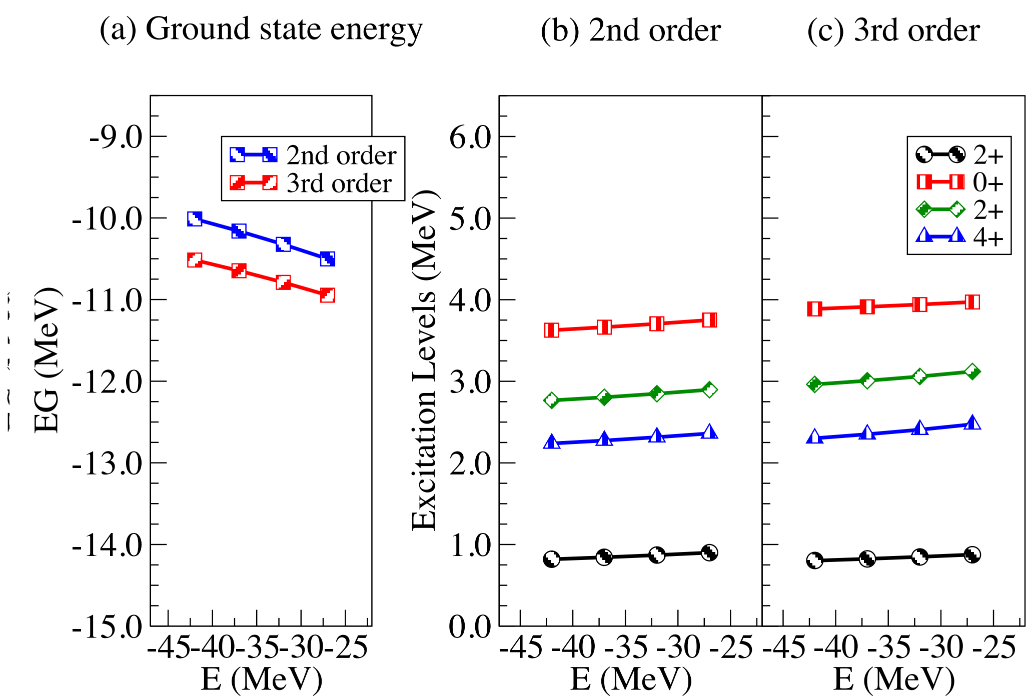
E_d3/2 = +1.6466 MeV

E_s1/2 = -3.1635 MeV

E_d5/2 = -3.9478 MeV



hw = 14



E=0 corresponds to the lowest pole of Q-box

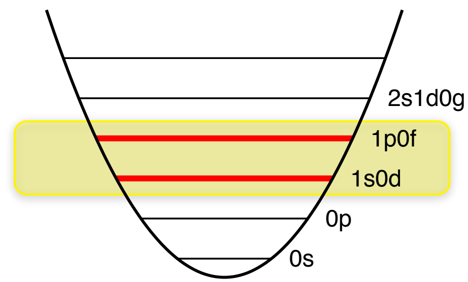
N3LO
Vlowk (cutoff=2.0 fm^-1, sharp cutoff)

*V*eff for *sdpf*-shell

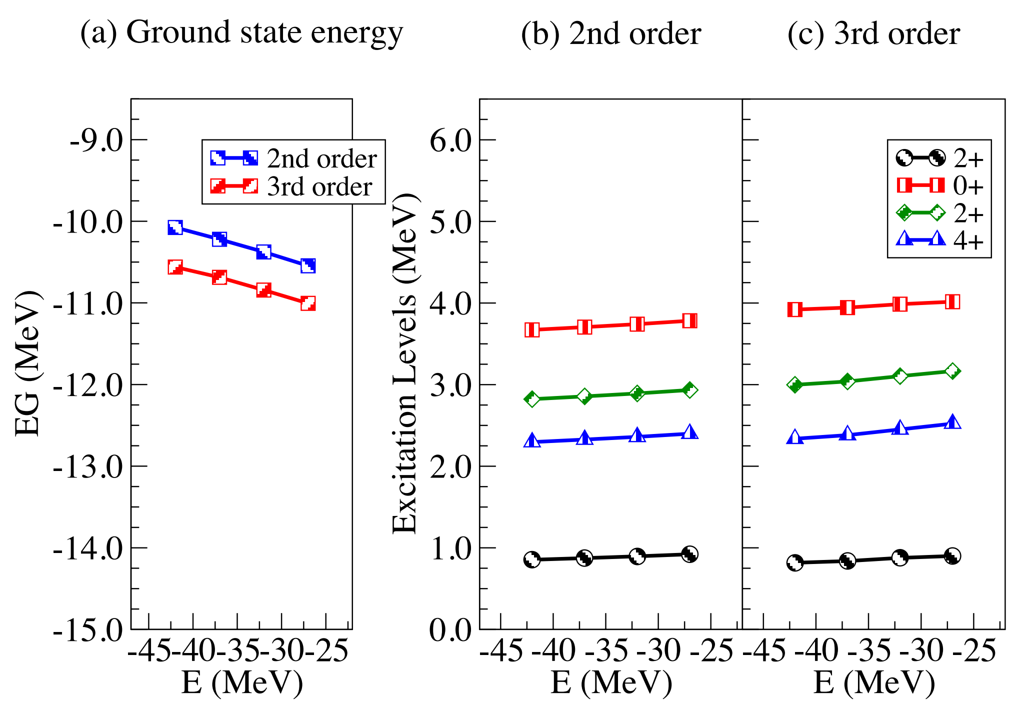
E-independence of the EKK method

O18 with respect to O16

Empirical sp energies from SDPF-M
E_d3/2 = +1.6466 MeV
E_s1/2 = -3.1635 MeV
E_d5/2 = -3.9478 MeV
E_pf =3.10 MeV



hw = 14



E=0 corresponds to the lowest pole of Q-box

N3LO
Vlowk (cutoff=2.0 fm^-1, sharp cutoff)

Conclusion and future perspective

- A new method to derive the effective interaction for the shell model in **non-degenerate** model space is constructed (EKK method)
  - Diagrammatic approach based on *time-dependent perturbation theory* ***exactly*** corresponds to the *formal theory*
  - *sd*-shell and *sdpf*-shell effective interaction is calculated as test calculations
    - Up to 2^{nd} and 3^{rd} order in interaction

- ***Arbitrary parameter E*** in introduced
  - The results should *not* depend on E if the Q-box is calculated exactly
  - E-independence is a measure for the accuracy of the calculation
    - better in 3^{rd} order than 2^{nd} order