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

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Motivation

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

Nuclear force in nuclear medium

Nuclear properties

empirically or microscopically derived
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.
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Effective interaction for the shell model

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- 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

If the model space is not degenerated...

- Divergent or nearly divergent
- Strong non-Hermiticity

\[
\frac{V_{cph}V_{hdpb}}{\epsilon_d - \epsilon_b - \epsilon_p + \epsilon_h}
\]
3. Review of MBPT
(Kuo-Krenciglowa method)
Formal theory

Definitions and setups

\[ H|\Psi_\lambda\rangle = E_\lambda|\Psi_\lambda\rangle \quad P^2 = P, \quad P + Q = 1 \quad \lambda = 1, 2, \cdots, d, \cdots, n \]
\[ P|\Psi_i\rangle = |\Phi_i\rangle \quad \omega|\Phi_i\rangle = Q|\Psi_i\rangle \quad Q\omega P = \omega \quad i = 1, 2, \cdots, d \]
\[ \mathcal{H} = e^{-\omega}He^{\omega} \quad \text{(Similarity transf. : yields the same eigenvalues as original Hamiltonian H)} \]

Decoupling equation

\[ 0 = QHP = QVP - \omega PHP + QHQ\omega - \omega PVQ\omega \]

Effective Hamiltonian

\[ H_{\text{eff}} = PHP \quad H_{\text{eff}}|\Psi_i\rangle = E_i|\Psi_i\rangle \]
\[ V_{\text{eff}} = PV P + PVQ\omega, \quad H_{\text{eff}} = PHP + PVQ\omega \]

Veфф: Effective interaction defined in purely in P-space

**Problem**: How can we obtain \( \omega \) which fulfill the decoupling equation?
Kuo-Krenciglowa (KK) method


Iterative solution of decoupling equation

\[ 0 = QHP = QVP - \omega PHP + QHQ\omega - \omega PVQ\omega \]

\[ PH_0P = \epsilon_0 \]

(Degenerate model space is assumed)

\[ (\epsilon_0 - QHQ)\omega = QVP - \omega PVP - \omega PVQ\omega \]

\[ \omega = \frac{1}{\epsilon_0 - QHQ} QVP - \frac{1}{\epsilon_0 - QHQ} \omega V_{\text{eff}} \]

\[ V_{\text{eff}} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0) \{ V_{\text{eff}} \}^k \]

Solve this equation iteratively

Q-box

\[ \hat{Q}(\epsilon) = PV P + PV Q \frac{1}{\epsilon - QHQ} QVP \quad \hat{Q}_k(\epsilon_0) = \frac{1}{k!} \left\{ \frac{d^k \hat{Q}}{d\epsilon} \right\}_{\epsilon = \epsilon_0} \]

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4. EKK method
Extended KK (EKK) method

Decoupling equation

\[
0 = QHP = QVP - \omega PHP + QHQ\omega - \omega PVQ\omega
\]

\[
(E - QHQ)\omega = QVP - \omega P\tilde{H}P - \omega PVQ\omega
\]

arbitrary constant energy parameter

\[
\omega = \frac{1}{E - QHQ} QVP - \frac{1}{E - QHQ} \omega \tilde{H}_{\text{eff}}
\]

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

\[
\tilde{H} = H - E \\
H_{\text{BH}}(\epsilon) = PHP + PVQ \frac{1}{\epsilon - QHQ} QVP
\]

• 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)

\[ V_{\text{eff}} = \hat{Q}(\epsilon_0) - \hat{Q}'(\epsilon_0) \int \hat{Q}(\epsilon_0) + \hat{Q}'(\epsilon_0) \int \hat{Q}(\epsilon_0) \int \hat{Q}(\epsilon_0) + \cdots \]

\[ V_{\text{eff}} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0) \{ V_{\text{eff}} \}^k \]

- 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
$H = \begin{pmatrix} PHP & PHQ \\ QHP & QHQ \end{pmatrix} = \begin{pmatrix} PH_0P & 0 \\ 0 & QH_0Q \end{pmatrix} + \begin{pmatrix} PVP & PVQ \\ QVP & QVQ \end{pmatrix}$

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

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

- 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

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

**KK method**

Unperturbed Hamiltonian

\[ H_0 = \sum_i \epsilon_i a_i^\dagger a_i \]

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

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

**EKK method**

Unperturbed Hamiltonian

\[ H_0 = PeP + Q \sum_i (\epsilon_i a_i^\dagger a_i) Q \]

\[ P = \sum_{i=1}^d |\Phi_i\rangle \langle \Phi_i| = \sum_{i,j=\text{act}} a_i^\dagger a_j^\dagger |c\rangle \langle c|a_j a_i, \ Q = 1 - P \]

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

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

\[
\begin{align*}
|a\rangle &\quad |b\rangle \\
|p_1\rangle &\quad |p_2\rangle \\
|c\rangle &\quad |d\rangle \\
\end{align*}
\]

\[ \langle c| a_b a_a H_1 \int_{-\infty}^0 dt_1 H_1(t_1) a_d^\dagger a_b^\dagger |c\rangle \]

\[ t=0 \quad \rightarrow \quad \langle c| a_b a_a \left( a_d^\dagger a_b^\dagger V_{ab,p_1 p_2} a_p a_p a_{p_1} \right) \int_{-\infty}^0 dt_1 \left( e^{iH_0 t_1} a_{p_1}^\dagger a_{p_2}^\dagger V_{p_1 p_2,c} a_d a_c e^{-iH_0 t_1} \right) a_c^\dagger a_d^\dagger |c\rangle \]

\[ = \langle c| a_b a_a \left( a_d^\dagger a_b^\dagger V_{ab,p_1 p_2} a_p a_p a_{p_1} \right) \int_{-\infty}^0 dt_1 \left( e^{iH_0 t_1} a_{p_1}^\dagger a_{p_2}^\dagger V_{p_1 p_2,c} a_d a_c \right) a_c^\dagger a_d^\dagger |c\rangle e^{-iEt_1} \]

\[ = \frac{V_{ab,p_1 p_2} V_{p_1 p_2,c} a_d a_c}{E - \epsilon_{p_1} - \epsilon_{p_2}} \]

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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)

Examples of the diagrams included in Q-box

Pure two-body contribution

One-body to two-body contribution
E-independence of the EKK method

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

\[ \tilde{H} = H - E \]

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
$V_{\text{eff}}$ for $sd$-shell
Empirical sp energies from USD
E_{d3/2} = +1.6466 MeV
E_{s1/2} = -3.1635 MeV
E_{d5/2} = -3.9478 MeV

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

N3LO
V_{lowk} (cutoff=2.0 fm^{-1}, sharp cutoff)
Veff 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

(a) Ground state energy
(b) 2nd order
(c) 3rd order

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