# Effective interactions of nuclei

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## **Construction of "Bridges"**



Naofumi Tsunoda (CNS UT) Derivation of

**Derivation of Veff and its application** 

- Understand effective interaction of nuclei
- Theory of "renormalization" of nuclear force
- Folded diagram method
- Current status of this line of research

- History of shell model calculation and effective interaction
  - Various effective interactions for shell model
- What is effective interaction?
  - Toy model
- Formal theories of effective interaction
  - KK method



Review of time-dependent perturbation theory

- Interaction picture
- Dyson equation
- Folded diagram method
  - Factorization
- Implementation

- Extended Kuo-Krenciglowa method
- Recent application of MBPT
  - Island of inversion
  - Comparison to latest experiments
  - Open problems

## Nuclear force in medium

realistic nucleon-nucleon interaction

- two-body interaction in vacuum
- "bare" NN interaction
- determined by scattering experiment
- Non-central nature
- Not applicable to nuclear many-body problem directly



- two-body interaction in nuclear medium
- "renormalized" NN interaction
- designed for chosen degrees of freedom
- determined by shell model fitting or microscopic theory
- effective Non-central nature



## History of shell model and nuclear experiment

Naofumi T	sunoda (CNS UT)	Derivation of Veff a	and its a	pplication	8 /39
numerio	cal capability	shell model		exp	periment
			1910	Discove	ery of nucleus
			1930	Inventio	n of Cyclotron
		Yukawa theory			
		birth of shell model	1950	magn	etic moment 
10~100		model independent particle shell model		mass	mesurement
	single f7/2 shell	interacting shell	1960	exci spin-pa	tation states ritv assignment
		KK method Kuo-Brown	1970		
100	full sd-shell	KB3G interaction USD interaction			
108	full pf-shell	GXPF1 interaction		nucle RI be	eosynthesis am facilites
IO''~I( large scal	le shell model calculation	SDPF-M interaction	2000	neut c	ron/proton drip-line
	<b>7</b> 23		2010	neu	utron halo

## **Shell evolution**



Shell structure is changed drastically with the proton number  $\rightarrow$  key ingredient is effective nucleon-nucleon interaction

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#### **Nuclear chart**



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#### Early stage of effective interaction to nuclei

[1] T. T. S. Kuo and G. E. Brown, Nucl. Phys. A 114, 241 (1968).



Fig. 3. Energy levels of <sup>42</sup>Ca and <sup>42</sup>Sc calculated with G and  $G_{3p1h}$ . The experimental level schemes at from refs. <sup>13, 14</sup>).

- G-matrix from Hamada-Jonston int.
- 2hw excitation
- 3p1h diagram included

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#### Early stage of effective interaction to nuclei

[1] H. M. Sommermann, et al., Physical Review C 23, 1765 (1981).







FIG. 7. Spectrum of  ${}^{18}$ F (T = 0). See explanation of Fig. 6.

G-matrix from Hamada-Jonston int.

22 hw excitation

0

- 3p1h diagram included
- with folded diagrams



## G-matrix + MBPT + fit

[1] B. A. Brown et al., Annals of Physics 182, 191 (1988).



- Famous USD interaction
- Kuo-Brown interaction is modified (called renormalized G-matrix)

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#### MBPT for single major shell

[1] M. Hjorth-Jensen et al., Phys. Rep. 261, 125 (1995).



Fig. 42. The low-lying spectra for <sup>18</sup>O with the Bonn C potential.

- G-matrix from Bonn A, B, C pot.
- many hw excitation
- Ind, 3rd order and folded diagrams

[1] Y. Utsuno et al., Phys. Rev.C C60, 054315 (1999).



FIG. 6. Yrast levels of Ne (top), Mg (center), and Si (bottom) isotopes. The filled (open) triangles, diamonds are the experimental (calculated)  $2_1^+$  and  $4_1^+$  levels, respectively. The crosses mean  $E_x(2_1^+)$  calculated by the *sd*-shell model.



FIG. 8. Average number of neutrons in the pf shell subtracted by the corresponding number in the normal (i.e., filling) configuration. The triangles, diamonds, and circles stand for the values of Ne, Mg, and Si isotopes, respectively. The solid line denotes the corresponding value of Ne and Mg isotopes as predicted by the "island of inversion" of [11].

- sdpf-m int.
- island of inversion
- N=20 gap
- sd+pf shell



[1] E. Caurier, et al., Phys. Rev. C 90, 014302 (2014).

FIG. 11. (Color online) Excitation energies of the first  $2^+$  states in the silicon isotopes (see caption of Fig. 6).

FIG. 12. (Color online) Comparison between experiment and theory for the most important low lying states in <sup>30</sup>Mg, <sup>32</sup>Mg, and <sup>34</sup>Si.

- sdpf-U-mix int.
- merging island of inversion and N=28 gap
- sd+pf shell



[1] E. Caurier, et al., Phys. Rev. C 90, 014302 (2014).

FIG. 11. (Color online) Excitation energies of the first  $2^+$  states in the silicon isotopes (see caption of Fig. 6).

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- sdpf-U-mix int.
- merging island of inversion and N=28 gap
- sd+pf shell

#### [1] Y. Tsunoda et al., Phys. Rev. C 89, 031301 (2014).



FIG. 3. (Color online) Potential energy surfaces (PES) of Ni isotopes, coordinated by usual  $Q_0$  and  $Q_2$  (or  $\gamma$ ). The energy relative to the minimum is shown by contour plots. Circles on the PES represent shapes of MCSM basis vectors (see the text).

- pf-g9/2-d5/2-shell
- Ni isotopes and shape transition
- Invention of T-plot

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#### [1] T. Togashi et al., Phys. Rev. Lett. 117, 172502 (2016).



TABLE I. Model space for the shell model calculation.

proton orbit	magic number	neutron orbit	
-		$1f_{7/2}, 2p_{3/2}$	
	82		
-		$0h_{11/2}$	
$0g_{7/2}, 1d_{5/2,3/2}, 2s_{1/2}$		$0g_{7/2}, 1d_{5/2,3/2}, 2s_{1/2}$	
	50		
0g <sub>9/2</sub>		$0g_{9/2}$	
$0 f_{5/2}, 1 p_{3/2,1/2}$		-	

Large model space

- sudden change of 2+ and 0+ level w.r.t. N
- Quantum phase transition

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#### Shell model effective interactions

- Attempt to obtain effective interactions for the shell model calculation first done by Kuo and Brown in 1968.
- There exists many effective interactions for shell model calculation
- Recent calculations mainly based on the effective interaction obtained by fit
- Fitting usually done on top of so-called G-matrix or MBPT.

#### What is "effective" interaction



- Solve same physics for chosen degrees of freedom
- Same d eigen values and eigen vectors
- Typically low energy physics

#### What is "effective" interaction?

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 5 \end{pmatrix}$$
 3x3 matrix

Eigenvalues and eigenvectors

$$\begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} = \begin{pmatrix} -1.08 \\ 0.88 \\ 5.19 \end{pmatrix} \begin{pmatrix} 0.92 \\ -1.00 \\ 0.038 \end{pmatrix} \begin{pmatrix} -1.00 \\ -0.88 \\ 0.20 \end{pmatrix} \begin{pmatrix} 0.16 \\ 0.22 \\ 1.00 \end{pmatrix}$$

Suppose if we are interested in only lowest two states.

P-space 
$$\left\{ \begin{pmatrix} 1\\ 0 \end{pmatrix}, \begin{pmatrix} 0\\ 1 \end{pmatrix} \right\}$$

$$PVP = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} -1.0 \\ 1.0 \end{pmatrix} \qquad \begin{pmatrix} 1.0 \\ -1.0 \end{pmatrix} \begin{pmatrix} -1.0 \\ -1.0 \end{pmatrix}$$

Different eigenvalues and eigenenergies

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Then, what is the interaction which yields the same eigenvalues and eigenvectors?

 $\begin{pmatrix} 1.2 * 10^{-5} & 1 - 1.5 * 10^{-5} \\ 1 - 0.48 * 10^{-1} & -0.19 \end{pmatrix}$  2x2 matrix  $\begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} -1.08 \\ 0.88 \end{pmatrix} \quad \begin{pmatrix} 0.92 \\ -1.00 \end{pmatrix} \begin{pmatrix} -1.00 \\ -0.88 \end{pmatrix}$ 

Same eigenvalues and eigenvectors for lowest 2 states.

—> different from PVP, but quite similar.
What was the point?



## Separation of the scale



- If the P-space are well separated from Q-space, renormalized matrix is not far from PVP
- Non hermiticity is not large



#### Model space, P-space

Hamiltonian

$$H = H_0 + V, \quad H_0 |\phi_i\rangle = E_i |\phi_i\rangle$$

Projection operator

 $[P, H_0] = [Q, H_0] = 0. \qquad P^2 = P, \quad Q^2 = Q$ PQ = QP = 0,[P, Q] = 0.





Ρ

#### Easy way to formulate

$$\begin{pmatrix} PHP & PVQ \\ QVP & QHQ \end{pmatrix} \begin{pmatrix} |\phi_{\lambda}\rangle \\ |\rho_{\lambda}\rangle \end{pmatrix} = E_{\lambda} \begin{pmatrix} |\phi_{\lambda}\rangle \\ |\rho_{\lambda}\rangle \end{pmatrix},$$

$$|\rho_{\lambda}\rangle = (E_{\lambda} - QHQ)^{-1}QVP|\phi_{\lambda}\rangle$$

$$|\phi_{\lambda}\rangle = (E_{\lambda} - PHP)^{-1}PVQ|\rho_{\lambda}\rangle.$$

$$\begin{pmatrix} PHP - \frac{1}{E_{\lambda} - QHQ}QVP \end{pmatrix} |\phi_{\lambda}\rangle = E_{\lambda}|\phi_{\lambda}\rangle$$

$$\begin{pmatrix} QHQ - \frac{1}{E_{\lambda} - PHP}PVQ \end{pmatrix} |\rho_{\lambda}\rangle = E_{\lambda}|\rho_{\lambda}\rangle.$$

$$\Psi_{\lambda} \rangle = \begin{pmatrix} \mathsf{C}_{1} \\ \vdots \\ \mathsf{C}_{\mathsf{D}} \\ \mathsf{C}_{\mathsf{D}+1} \\ \vdots \\ \mathsf{C}_{\mathsf{N}} \end{pmatrix} = |\phi_{\lambda}\rangle$$

Bloch-Horowitz Hamiltonian

$$H_{\rm BH}(E) = PHP + PVQ \frac{1}{E - QHQ} QVP.$$
$$H_{\rm BH}(E_{\lambda}) |\phi_{\lambda}\rangle = E_{\lambda} |\phi_{\lambda}\rangle, \quad \lambda = 1, \cdots, D.$$

#### Unsatisfactory because HBH depends on E.

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PHP	PVQ	
QVP	QHQ	

What we want to know is energy independent Hamiltonian which satisfies

$$H_{\text{eff}}|\phi_i\rangle = E_i|\phi_i\rangle, \quad i = 1, \cdots, d.$$

IF we know true eigenstates and eigenenegies, we can formulate Heff immediately as follows,

$$H_{\text{eff}} = \sum_{i=1}^{d} |\phi_i\rangle E_i \langle \tilde{\phi}_i |, \qquad \langle \tilde{\phi}_i | \phi_j \rangle = \delta_{ij}$$

Bi-orthogonal basis is used because  $|\phi\rangle$  does not span whole P-space in general.

-> non Hermitian Heff (more later)



#### How to find the Heff : decoupling equation

Similarity transformation  $\mathcal{H} = e^{-\omega} H e^{\omega}, \quad Q \omega P = \omega.$ 

Decoupling condition

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



 $H_{\rm eff} = P\mathcal{H}P$  $V_{\rm eff} = PVP + PVQ\omega.$ 

#### Next: Solve non-linear equation.

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#### Formal solution of decoupling equation (KK method)

Assumption: the model space is degenerate

 $PH_0P = \epsilon_0P.$ 

#### **Decoupling equation**

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

A solution for this equation

$$\begin{aligned} (\epsilon_0 - QHQ)\omega &= QVP - \omega PVP - \omega PVQ\omega. \\ \omega &= \frac{1}{\epsilon_0 - QHQ} \left( QVP - \omega \left( PVP + PVQ\omega \right) \right) \\ &= \frac{1}{\epsilon_0 - QHQ} \left( QVP - \omega V_{\text{eff}} \right), \end{aligned}$$

Solve this by iteration

$$\frac{Q-box:}{\hat{Q}(E) = PVP + PVQ} \frac{1}{E - QHQ} QVP,$$

$$\hat{Q}_k(E) = \frac{1}{k!} \frac{d^k \hat{Q}(E)}{dE^k}.$$

$$\blacktriangleright V_{\text{eff}}^{(n)} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0) \{V_{\text{eff}}^{(n-1)}\}^k.$$

Iterative equation for deriving the Effective interaction for degenerate model space

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### What is Q-box ?



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#### **Conceptual drawing of Heff**

Nuclear force in vacuum



#### in-medium correction

core polarization (3p1h)



#### Central force of AV8' potential



 $V_C = v_1(r) + (\sigma_1 \cdot \sigma_2)v_2(r) + (\tau_1 \cdot \tau_2)v_3(r) + (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)v_4(r).$ 

- Strong short range repulsion.
- High-momentum component.
- Can it be renormalized to low momentum int.?



#### **Vlowk interaction**

Lippmann-Schwinger equation

$$T(k',k;k^2) = V_{NN}(k',k) + \frac{2}{\pi} \mathcal{P} \int_0^\infty \frac{V_{NN}(k',p)T(p,k;k^2)}{k^2 - p^2} p^2 dp$$

Low-momentum interaction  $V_{\text{lowk}}$  which preserves the HOS T-matrix

$$T(k',k;k^2) = V_{\text{low}k}(k',k) + \frac{2}{\pi} \mathcal{P} \int_0^{\Lambda} \frac{V_{\text{low}k}(k',p)T(p,k;k^2)}{k^2 - p^2} p^2 dp.$$

RG equation of  $V_{\text{lowk}}$  equation with respect to cutoff parameter  $\Lambda$ 

$$\longrightarrow \quad \frac{\mathrm{d}V_{\mathrm{low}k}(k',k)}{\mathrm{d}\Lambda} = \frac{2}{\pi} \frac{V_{\mathrm{low}k}(k',\Lambda)T(\Lambda,k;\Lambda^2)}{1-(k^2/\Lambda^2)}.$$



- Decouple low-momentum and high-momentum part
- Preserve physical observable and low-momentum wave function
- Remove repulsive core

#### Implementation of Vlowk interaction

## Usu this equation instead of RG equation $H_{\text{eff}} = \sum_{i=1}^{d} |\phi_i\rangle E_i \langle \tilde{\phi}_i |, \qquad \langle \tilde{\phi}_i | \phi_j \rangle = \delta_{ij}$

$$V_{lowk} = \sum_{k < k_F} |\phi_k\rangle E_k \langle \tilde{\phi_k}| - T$$



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#### Non hermiticity

$$V_{\rm eff} = PVP + PVQ\omega.$$

$$(P + \omega^{\dagger}\omega)H_{\rm eff} = H_{\rm eff}^{\dagger}(P + \omega^{\dagger}\omega).$$

Cholesky decomposition: lower triangular matrix L

$$P + \omega^{\dagger}\omega = LL^{\dagger}.$$
  

$$L^{-1}H_{\text{eff}}^{\dagger}L = L^{\dagger}H_{\text{eff}}(L^{\dagger})^{-1} = \left(L^{-1}H_{\text{eff}}^{\dagger}L\right)^{\dagger}$$
  

$$H_{\text{eff}}^{her} = L^{\dagger}H_{\text{eff}}(L^{\dagger})^{-1}.$$

If  $\omega$  is enough small,  $H^{her}_{eff} \rightleftharpoons H_{eff}$ 


# Many body problem

Hamiltonian in second quantized form

$$\begin{split} H &= H_0 + V \\ &= \sum_{d} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{2} \sum V_{\alpha\beta,\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}, \\ P &= \sum_{i} |\phi_i\rangle \langle \phi_i| \\ |\phi_i\rangle &= \sum a_{\lambda}^{\dagger} a_{\gamma}^{\dagger} |c\rangle. \end{split}$$



In Schrodinger picture

 $H|\Psi_n\rangle = E_n|\Psi_n\rangle$ 



# **Interaction picture**

## Interaction picture is suitable for perturbation theory

$$\begin{split} H_{1}^{I}(t) &= e^{-iH_{0}t}H_{1}e^{iH_{0}t} \\ |\Psi^{I}(t)\rangle &= e^{-iH_{0}t}|\Psi^{S}(t)\rangle \\ \hat{O}^{I}(t) &= e^{-iH_{0}t}\hat{O}e^{iH_{0}t}, \end{split}$$

Heisenberg formula

$$\frac{d}{dt}\hat{O}^{I}(t) = -i[H_0, O]$$

Creation and annihilation operators

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# **Dyson equation**

Time-development of w.f. in interaction picture

$$i\frac{d}{dt}|\Psi(t)\rangle = H_1(t)|\Psi(t)\rangle$$

$$|\Psi(t)\rangle = |\Psi(t_0)\rangle + (-i)\int_{t_0}^{\bullet} dt' H_1(t)|\Psi(t')\rangle$$

Defining time-development operator

 $|\Psi(t)\rangle = U(t,t')|\Psi(t')\rangle$ 

Iterative solution: Dyson equation

$$U(t,t') = \lim_{\epsilon \to 0} \lim_{t' \to -\infty(1-i\epsilon)} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^t dt_1 \int_{t'}^t dt_2 \cdots \int_{t'}^t dt_n T[H_1(t_1)H_1(t_2)\cdots H_1(t_n)].$$

# **Diagrammatic expression**

$$\begin{split} U(0,-\infty)a_a^+a_b^+|c\rangle \\ = & \left( \begin{array}{c} + & 0 \\ + & 0 \\ + & 1 \end{array} \right) = a_e^+a_f^+|c\rangle \times \lim_{t' \to -\infty(1+i\epsilon)} (-i)^2 \int_{t'}^0 dt_1 \int_{t'}^{t_1} dt_2 \\ & e^{-i(\epsilon_e + \epsilon_d - \epsilon_e - \epsilon_f)t_1} \\ & e^{-i(\epsilon_a + \epsilon_b - \epsilon_e - \epsilon_d)t_2} \\ & \times V_{abcd}V_{cdef} \\ & = a_e^+a_f^+|c\rangle \times \lim_{t' \to -\infty(1+i\epsilon)} (-i) \int_{t'}^0 dt_1 e^{-i(\epsilon_e + \epsilon_d - \epsilon_e - \epsilon_f)t_1} \\ & \frac{e^{-i(\epsilon_a + \epsilon_b - \epsilon_e - \epsilon_d)t_1}}{-i(\epsilon_a + \epsilon_b - \epsilon_e - \epsilon_d)} \\ & \times V_{abcd}V_{cdef} \\ & = a_e^+a_f^+|c\rangle \times \frac{1}{\epsilon_a + \epsilon_b - \epsilon_e - \epsilon_f} \frac{1}{\epsilon_a + \epsilon_b - \epsilon_e - \epsilon_d} \times V_{abcd}V_{cdef} \end{split}$$

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# **Time-dependent perturbation theory**



Parent states: "projection" of true eigen states to P-space  $\langle \rho_{\lambda} | P \Psi_{\mu} \rangle = 0$   $(\lambda \neq \mu = 1, 2, \cdots, D).$ 

-> Because of i  $\varepsilon$  term the **lowest** eigenstates survive.

$$\frac{|\Psi_{\lambda}\rangle}{\langle \rho_{\lambda}|\Psi_{\lambda}\rangle} = \lim_{\epsilon \to 0} \lim_{t' \to -\infty(1-i\epsilon)} \frac{U(0,t')|\rho_{\lambda}\rangle}{\langle \rho_{\lambda}|U(0,t')|\rho_{\lambda}\rangle} \longrightarrow H\frac{U(0,-\infty)|\rho_{\lambda}\rangle}{\langle \rho_{\lambda}|U(0,-\infty)|\rho_{\lambda}\rangle} = E_{\lambda}\frac{U(0,-\infty)|\rho_{\lambda}\rangle}{\langle \rho_{\lambda}|U(0,-\infty)|\rho_{\lambda}\rangle}$$

Of course we do not know true eigenstates  $|\Psi\rangle$  and therefore its projection  $|\rho\rangle$ .

Being  $|\psi\rangle$  known P-space basis vectors, we can formally write down as

$$|\rho_{\lambda}\rangle = \sum_{\alpha=1}^{a} C_{\alpha}^{(\lambda)} |\psi_{\alpha}\rangle.$$

λ

Then we obtain,

$$\sum_{\alpha=1}^{D} C_{\alpha}^{(\lambda)} H \frac{U(0,-\infty)|\psi_{\alpha}\rangle}{\langle \rho_{\lambda}|U(0,-\infty)|\rho_{\lambda}\rangle} = \sum_{\beta=1}^{D} C_{\beta}^{(\lambda)} E_{\lambda} \frac{U(0,-\infty)|\psi_{\beta}\rangle}{\langle \rho_{\lambda}|U(0,-\infty)|\rho_{\lambda}\rangle}.$$

## $HU(0, -\infty) \cong Heff$

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# What we know so far



# Factorization

## $U|\psi$ > can be factorized to several pieces

$$U(0,-\infty)|\psi_{\alpha}\rangle = U_{V}(0,-\infty)a_{i}^{\dagger}a_{j}^{\dagger}|c\rangle \times U(0,-\infty)|c\rangle,$$

$$U(0,-\infty)|c\rangle = U_{Q}(0,-\infty)|c\rangle \times \langle c|U(0,-\infty)|c\rangle,$$

- V: Valence linked
- Q: terminate as Q-space state
- C: core state





# Factorization

 $U_V(0,-\infty)|\psi_{\alpha}\rangle = |\chi_P\rangle + |\chi_Q\rangle.$ 

P: terminate as P-space state Q: terminate as Q-space state



# Folded diagrams

To factorize further, define folded diagrams as follows:



Then, we can factorize as follows,

$$\begin{split} |\chi_Q\rangle &= \left| \left( \begin{matrix} \# \\ \textcircled{0} \end{matrix}\right) - \begin{matrix} \# \\ \textcircled{0} \end{matrix}\right) \int \begin{matrix} \oplus \\ \textcircled{0} \end{matrix}\right) + \begin{matrix} \# \\ \textcircled{0} \end{matrix}\right) \int \begin{matrix} \oplus \\ \textcircled{0} \end{matrix}\right) \int \begin{matrix} \oplus \\ \textcircled{0} \end{matrix}\right) + \begin{matrix} \cdots \\ \cdots \end{matrix}\right| |\chi_P\rangle \\ U_V(0, -\infty) |\psi_\alpha\rangle &= \sum_{\beta=1}^D U_{VQ}(0, -\infty) |\psi_\beta\rangle \langle \psi_\beta | U_V(0, -\infty) |\psi_\alpha\rangle. \end{split}$$

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# **Finally Heff**

Remember

$$\sum_{\alpha=1}^{D} C_{\alpha}^{(\lambda)} H \frac{U(0,-\infty)|\psi_{\alpha}\rangle}{\langle \rho_{\lambda}|U(0,-\infty)|\rho_{\lambda}\rangle} = \sum_{\beta=1}^{D} C_{\beta}^{(\lambda)} E_{\lambda} \frac{U(0,-\infty)|\psi_{\beta}\rangle}{\langle \rho_{\lambda}|U(0,-\infty)|\rho_{\lambda}\rangle}$$

Combining obtained knowledge,

 $U(0,-\infty)|\psi_{\alpha}\rangle = U_{Q}(0,-\infty)|c\rangle\langle c|U(0,-\infty)|c\rangle \times \sum_{\beta=1}^{d} U_{VQ}(0,-\infty)|\psi_{\beta}\rangle\langle\psi_{\beta}|U_{V}(0,-\infty)|\psi_{\alpha}\rangle$ 

$$\sum_{\gamma=1}^{d} b_{\gamma}^{\lambda} H U_{Q}(0, -\infty) |c\rangle U_{VQ}(0, -\infty) |\psi_{\gamma}\rangle = \sum_{\delta=1}^{d} b_{\delta}^{\lambda} E_{\lambda} U_{Q}(0, -\infty) |c\rangle U_{VQ}(0, -\infty) |\psi_{\gamma}\rangle$$

$$b_{\gamma}^{(\lambda)} = \sum_{\alpha=1}^{d} C_{\alpha}^{(\lambda)} \frac{\langle \psi_{\gamma} | U_{V}(0, -\infty) |\psi_{\alpha}\rangle \langle c | U(0, -\infty) |c\rangle}{\langle \rho_{\lambda} | U(0, -\infty) |\rho_{\lambda}\rangle}$$

Define linked pieces as follows,

 $U_{L}(0,-\infty)|\psi_{\alpha}\rangle \equiv U_{VQ}(0,-\infty)|\psi_{\alpha}\rangle U_{Q}(0,-\infty)|c\rangle,$   $\longrightarrow \sum_{\gamma=1}^{d} b_{\gamma}^{(\lambda)} \langle \psi_{\sigma} | HU_{L}(0,-\infty) | \psi_{\lambda} \rangle = E_{\lambda} | \psi_{\sigma} \rangle.$ Heff\_total



# Factorization and folded diagram method

$$\sum_{\gamma=1}^{d} b_{\gamma}^{(\lambda)} \langle \psi_{\sigma} | HU_{L}(0, -\infty) | \psi_{\lambda} \rangle = E_{\lambda} | \psi_{\sigma} \rangle.$$
  
Heff\_total

Extract contribution of the core

$$PH_{\rm eff}P|\Psi_{\alpha}\rangle = (E_{\alpha} - E_{C})P|\Psi_{\alpha}\rangle$$

 $H_{\text{eff}} = \langle \psi_{\sigma} | (H_0(V) + H_1(V)) U_L(0, -\infty) | \psi_{\lambda} \rangle. \quad \text{V: valence linked}$ 



core







This is Q-box !  $\hat{Q}(E) = PVP + PVQ \frac{1}{E - QHQ} QVP$ ,

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# Folded diagrams and energy derivative



Folded diagrams can be calculated by energy derivative if the model space is degenerate

$$\rightarrow V_{\text{eff}}^{(n)} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0) \{V_{\text{eff}}^{(n-1)}\}^k.$$
 Final expression



# **Q-box expansion**



Diagrams appearing in 2nd order

# **Example of Q-box calculation**



 $= \sum_{p,h} \frac{V_{ch,ap} V_{pd,hb}}{\epsilon_b - \epsilon_d - \epsilon_p + \epsilon_h}$ 



$$= \sum_{p_1,p_2} \frac{V_{cd,p_1p_2}V_{p_1p_2,ab}}{\epsilon_a + \epsilon_b - \epsilon_{p_1} - \epsilon_{p_2}}$$

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Diagrams appearing in 3rd order

# Summary of folded diagram method



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# **EKK code algorithm**



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# **MPI+openMP** scaling

Test case: sdpf-shell 13major shells oakforest (64 core, max 2048 nodes)



# of nodes ~ # of TBMEs
nice scaling



# Model space and shell model Hamiltonian

	Lower	Upper
	shell	shell
Lower shell	Plenty of exp. data	Few exp. data
Upper shell	Few exp. data	Plenty of exp. data

ex) Phenom. int.

- USD int.
- gxpf1
- KB3
- Cohen-Kurath

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- sdpf-m
- sdpf-U-mix

etc…

# Cross-shell mtx: difficult to fit to exp. data

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# **EKK method**







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### Effective interaction in non-degenerate model space

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# EKK method in a schematic model

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#### Multi-shell effective interactions

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**Background:** Effective interactions, either derived from microscopic theories or based on fitting selected properties of nuclei in specific mass regions, are widely used inputs to shell-model studies of nuclei. The commonly used unperturbed basis functions are given by the harmonic oscillator. Until recently, most shell-model calculations have been confined to a single oscillator shell like the *sd* shell or the *pf* shell. Recent interest in nuclei away from the stability line requires, however, larger shell-model spaces. Because the derivation of microscopic effective interesting has been limited to descent the delayerest them are both concentrated and mosting limit.

EKK method in nuclei

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### Divergent problem of Q-box in non-degenerate model space

(A)KK method requires assumption that the model space is **degenerate**(B)Naive perturbation theory leads a **divergence** in non-degenerate model space



Energy denominator is zero when  $\varepsilon_d - \varepsilon_b = \varepsilon_p - \varepsilon_h$  We need a theory which satisfies

- (a)The assumption of degenerate model space is **removed**
- (b)**Avoid** the divergence appearing in Q-box diagrams

→ EKK method as a re-summation scheme of KK method



## Decoupling equation for the EKK method (formal solution)

Decoupling equation

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

Introduce energy parameter E

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

### EKK solution of parameter E

$$\rightarrow \qquad \tilde{H}_{\text{eff}}^{(n)} = \tilde{H}_{\text{BH}}(E) + \sum_{k=1}^{\infty} \hat{Q}_k(E) \{\tilde{H}_{\text{eff}}^{(n-1)}\}^k,$$

$$H_{\rm BH}(E) = PHP + PVQ \underbrace{1}_{E} QVP.$$
  
$$\tilde{H}_{\rm eff} = H_{\rm eff} - E, \quad \tilde{H}_{\rm BH}(E) = H_{\rm BH}(E) - E,$$

Points:

1. Arbitrary energy parameter E is introduced

 $\rightarrow$  results do <u>not</u> depend on the choice of E

- 2. Veff is substituted by Heff
- 3. Q-box and its derivatives are not changed, but evaluated at E



# Extended KK method as a re-summation of the perturbative series

## **EKK** method

### KK method (conventional)

New parameter E (arbitrary parameter)  

$$H = H'_{0} + V'$$

$$= \begin{pmatrix} E & 0 \\ 0 & QH_{0}Q \end{pmatrix} + \begin{pmatrix} P\tilde{H}P & PVQ \\ QVP & QVQ \end{pmatrix}, \qquad H = H_{0} + V$$

$$= \begin{pmatrix} PH_{0}P & 0 \\ 0 & QH_{0}Q \end{pmatrix} + \begin{pmatrix} PVP & H \\ QVP & QVP \end{pmatrix}$$

$$H_{BH}(E) = PHP + PVQ\frac{1}{E - QHQ}QVP, \qquad \hat{Q}(E) = PVP + PVQ\frac{1}{E - QHQ}QVP$$

$$\hat{Q}(E) = PVP + PVQ\frac{1}{E - QHQ}QVP$$

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

$$V_{eff}^{(n)} = \hat{Q}(\epsilon_{0}) + \sum_{k=1}^{\infty} \hat{Q}_{k}(\epsilon_{0}) \{V_{eff}^{(n-1)}\}^{k}.$$

- EKK method can be interpreted as a re-summation of KK method
- All the arguments are kept unchanged with the new division of the Hamiltonian

N. Tsunoda, K. Takayanagi, M. Hjorth-Jensen, and T. Otsuka, Phys. Rev. C 89, 024313 (2014).

Naofumi Tsunoda (CNS UT) Derivation of Veff and its application



# Example: EKK method avoids the divergences



• We can choose E to avoid divergence !

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- Note that the choice of E is arbitrary and should give the same result if the Q-box is calculated without any approximation.
- Inversely, E-dependence is a measure of error coming from the approximation



# **Diagrams appearing in EKK method**

 $(\Pi)$ 



(i)	$ \psi_i(t) angle$
(ii)	$\{a_a^{\dagger}a_p^{\dagger} c angle\}(t)$
(iii)	$\{a_a^{\dagger}a_b^{\dagger}a_p^{\dagger}a_h c angle\}(t)$

 $=e^{-iH'_{0}t}|\psi_{i}\rangle =e^{-iEt}|\psi_{i}\rangle P-\text{space}$   $=e^{-iH'_{0}t}\{a_{a}^{\dagger}a_{p}^{\dagger}|c\rangle\} =e^{-i(\epsilon_{a}+\epsilon_{p})t}a_{a}^{\dagger}a_{p}^{\dagger}|c\rangle, Q-\text{space}$   $=e^{-iH'_{0}t}\{a_{a}^{\dagger}a_{b}^{\dagger}a_{p}^{\dagger}a_{h}|c\rangle\} =e^{-i(\epsilon_{a}+\epsilon_{b}+\epsilon_{p}-\epsilon_{h})t}a_{a}^{\dagger}a_{b}^{\dagger}a_{p}^{\dagger}a_{h}|c\rangle, Q-\text{space}$ 

 $(\Pi)$ 

The argument of folded diagram is the same → derivatives indicate the folded diagram contribution



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# **Factorization theorem in EKK method**

Factorization theorem does not hold in EKK method naively



## E-depdence w and w/o non-perturbative correction



★ Non perturbative correction vanishes the E-dependecne
 ★ Optimum value of E

# <u>APPLICATION</u>

# VMU ~ renormalization persistency

Renormalization persistency of tensor force = tensor force **survives** renormalization treatment



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# VMU ~ renormalization persistency



FIG. 2 (color online). Diagrams for the  $V_{MU}$  interaction.

$$V_c = \sum_{S,T} f_{S,T} P_{S,T} \exp(-(r/\mu)^2),$$

Central force -> modeled by gaussian

- Tensor force -> bare  $\pi + \rho$  meson exchange
- widely used as effective int. for SM calc.

# Neutron-rich nuclei~ island of inversion



- E(2+)~1 MeV on N=20 indicate breaking of major shell gap
- Unified treatment of beyond and below the N=20 gap is necessary
- And this is one of many examples….

#### PHYSICAL REVIEW C 95, 021304(R) (2017)

### Exotic neutron-rich medium-mass nuclei with realistic nuclear forces

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We present the first application of the newly developed extended Kuo-Krenciglowa (EKK) theory of the effective nucleon-nucleon interaction to shell-model studies of exotic nuclei, including those where conventional approaches with fitted interactions encounter difficulties. This EKK theory enables us to derive an interaction that is suitable for several major shells (sd + pf in this work). By using such an effective interaction obtained from the Entem-Machleidt QCD-based  $\chi N^3$ LO interaction and the Fujita-Miyazawa three-body force, the energies, E2 properties, and spectroscopic factors of low-lying states of neutron-rich Ne, Mg, and Si isotopes are nicely described, as the first shell-model description of the "island of inversion" without fit of the interaction. The long-standing question as to how particle-hole excitations occur across the sd-pf magic gap is clarified with distinct differences from the conventional approaches. The shell evolution is shown to appear similarly to earlier studies.

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# **3N interaction (Δ-hole interaction)**



- Adding up effective 2N interaction derived from 3N interaction to EKK 2N effective interaction [1]
- This is one of the lowest order interaction from 3N force and for higher order we are working on…

[1] T. Otsuka, T. Suzuki, J. D. Holt, A. Schwenk, and Y. Akaishi, Phys. Rev. Lett. 105, 032501 (2010).

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Naofumi Tsunoda (CNS UT) Derivation of Veff and its application
## **3N interaction (momentum space integration)**

More modern and sophisticated choice of 3N



#### -> V<sub>lowk</sub> + V<sub>3N</sub> as starting point of MBPT

**Derivation of Veff and its application** 



### **Monopole interactions**



## **Island of inversion**

http://www.nndc.bnl.gov/nudat2/reCenter.jsp?z=12&n=20



- Around Ne and Mg region N=20 major gap disappears. (small 2+ energy for even-even nuclei, large deformation, etc…)
- · Ground state is consist of "inverse" configuration, i.e. intruder configuration
- $\cdot\,$  Can microscopic theory describe this disappearance of major magic number?

## Ground state energies and dripline



- Contribution of 3N force is significant in neutron-rich nuclei
- Predictions of dripline
- Combination of Microscopic theory and Large scale calc.

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### Shell structure in "island of inversion"





#### **Evolution of single particle states**

Effective single particle energies at N=20 isotones



3NF: general shift Tensor force: drive sd to pf gap



### Wave function of Mg isotopes



modest: shifting between two shells (e.g. pairing) abrupt : strong deformation

Abrupt excitation roughly corresponds to conventional 2p2h excitation model

### Effective single particle energies

Neutron(N=20)



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**Derivation of Veff and its application** 

### **Tensor force and 3N force**



- Enlarge the neutron <u>N=20 gap</u>
- $\pi d5/2 \nu f7/2(p3/2) = repulsive$
- $\pi d5/2 \nu d3/2 = attractive$
- Needed for doubly magic structure of Si34

- Enlarge the proton **Z=14 gap**
- Different physics, but needed for doubly magic structure of Si34 as well as tensor force

# **31Mg**



- onset of island of inversion
- ordering of levels reproduced
- positive=2hw dominanted
- negative=1hw dominated





- MBPT is the theory to construct the effective Hamiltonian starting from nuclear force.
- KK method or folded diagram method is introduced with formal theory and time-dependent perturbation theory
- <u>EKK method</u> is introduced to derive the effective interaction for the shell model which is applicable to multi-shell system.
- As an application of EKK method, the physics in the "island of inversion" is discussed in K-computer.
- EKK and 3N combination is the powerful tool to explore the wide area of the nuclear chart