素核宇宙融合 レクチャーシリーズ

第4回「原子核殻模型の基礎と応用」

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目次

- 核子の一粒子運動と原子核での殻構造
- 閉殻を仮定する(芯のある)殻模型計算の基礎
- 閉殻を仮定しない(芯のない)殻模型による 第一原理計算の概要
- モンテカルロ殻模型

Summary of 1st lecture

- Nucleon: Single-particle motion
- Independent Particle Model
 HO (central) potential + LS splitting
 Mayer-Jensen's magic #



Figure 2-23 Sequence of one-particle orbits. The figure is taken from M. G. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure*, p. 58, Wiley, New York, 1955.

Schematic picture of the single-particle potential

WS (HO) central potential + spin-orbit interaction



Conventional shell model



Shell-Model Hamiltonian

$$H = \sum_{i=1}^{N_{sps}} \epsilon_i n_i + \sum_{ijkl}^{N_{sps}} v_{ijkl} a_i^{\dagger} a_j^{\dagger} a_l a_k$$
$$n_i = a_i^{\dagger} a_i$$

 ϵ_i : Single-particle energy

 v_{ijkl} : Two-body matrix element (TBME)

• w/ some assumptions/approximations

Image of the shell-model Hamiltonian

• Hamiltonian:

$$H = \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i \neq j}^{A} V_{ij}$$

• Shell-model Hamiltonian:

$$H = \sum_{i=1}^{A} (T_i + U_i) + \frac{1}{2} \sum_{i \neq j}^{A} V_{ij} - \sum_{i=1}^{A} U_i$$

= $H_0 + H_1$

$$H_0 = \sum_{i=1}^{A} (T_i + U_i) \qquad \qquad H_1 = \frac{1}{2} \sum_{i \neq j}^{A} V_{ij} - \sum_{i=1}^{A} U_i$$

One-body (mean) field (一体場)

Residual interaction (残留相互作用; 摂動項)

Shell-model Hamiltonian

• Shell-model Hamiltonian

$$H = \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i \neq j}^{A} V_{ij}$$

$$= \sum_{i \leq A_c} T_i + \sum_{i < j \leq A_c} V_{ij} + \sum_{A_c < i} T_i + \sum_{i \leq A_c, A_c < j} V_{ij} + \sum_{A_c < i < j} V_{ij}$$

$$= H_c + H_v$$

$$H_c = \sum_{i \le A_c} T_i + \sum_{i < j \le A_c} V_{ij}$$

$$H_{v} = H_{0} + V_{v}$$

$$\downarrow \qquad \downarrow \qquad \downarrow$$

$$H = H_{0} + H_{1} \text{ (previous slide)}$$

$$H_0 = \sum_{A_c < i} (T_i + U_i) \quad U_j = \sum_{i \le A_c} V_{ij}$$

$$V_v = \sum_{A_c < i < j} V_{ij}$$

Shell-Model Hamiltonian



 ϵ_i : Single-particle energy

 v_{ijkl} : Two-body matrix element (TBME)

• w/ some assumptions/approximations

Procedure

- 1. Set the model space (valence space)
- 2. Get the <u>single-particle energies</u> (SPEs) from the exp. values
- 3. Compute the <u>two-body matrix elements</u> (TBMEs)
- 4. Diagonalize the Hamiltonian matrix (to get the <u>energy</u> <u>eigenvalues</u> & <u>eigenfunctions</u>) -> Configuration mixing
- 5. Calculate the <u>other obs.</u> (w) the w.f. obtained above)

 $H\Psi = E\Psi \qquad \qquad H = \sum_{i=1}^{N_{sps}} \epsilon_i n_i + \sum_{ijkl}^{N_{sps}} v_{ijk} a_i^{\dagger} a_j^{\dagger} a_l a_k$

Model space (single-particle states)

Single-particle orbits



$$N = 2n + | (+ 1)$$

= 1, 2, 3, ... J = | + s
(= 0, 1, 2, ...)

Orbital Angular Momentum	Symbol
I = 0	S
l = 1	р
l = 2	d
l = 3	f
I = 4	g
l = 5	h
I = 6	i

Figure 2-23 Sequence of one-particle orbits. The figure is taken from M. G. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure*, p. 58, Wiley, New York, 1955.

Model space for conventional shell model



Separation energy

• Separation energy: minimum energy to take a neutron/proton out



• Decrease suddenly after crossing the shell gap

Configuration mixing

Configuration mixing

• Configuration: pattern of occupation



Many-body wave function

• Single-particle Hamiltonian:

$$H_0 = \sum_{i=1}^A (T_i + U_i)$$

• Eigenvalue Equation:

 $H_0\psi_i = \epsilon_i\psi_i$

Single-particle w.f. Single-particle energy

• Many-body wave function:

$$\Psi_A \to \sum_{i}^{N_{sps}} x_i \mathcal{A} \left[\psi_1 \psi_2 \cdots \psi_A \right]$$

• Correlations are included by the configuration mixing.

Basis state

• Basis state (function):

$$\Phi = \frac{1}{\sqrt{n!}} \begin{vmatrix} \psi_a(\mathbf{r}_1) & \psi_a(\mathbf{r}_2) & \cdots & \psi_a(\mathbf{r}_{A_v}) \\ \psi_b(\mathbf{r}_1) & \psi_b(\mathbf{r}_2) & \cdots & \psi_b(\mathbf{r}_{A_v}) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_k(\mathbf{r}_1) & \psi_k(\mathbf{r}_2) & \cdots & \psi_k(\mathbf{r}_{A_v}) \end{vmatrix} \qquad A_v = A - A_c$$

$$A_v \qquad \qquad A_v \qquad \qquad A_v \qquad \qquad A_v \qquad \qquad A_v \qquad A_v \qquad \qquad A_v = A - A_c$$

$$A_v \qquad \qquad A_v = A - A_c$$

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$$A_v \qquad A_v \qquad A_v = A - A_c$$

$$A_v = A - A - A_c$$

$$A_v = A - A - A_c$$

$$A_v = A - A - A - A - A$$

$$A_v = A - A - A$$

Eigenvalue Equation

- Many-body wave function: $\Psi = \sum_{k=1}^{N_b} x_k \Phi_k = x_1 \Phi_1 + x_2 \Phi_2 + \dots + x_{N_b} \Phi_{N_b} \quad N_b : \text{#(basis)}$
- Eigenvalue equation:

$$H_{v}\Psi = E\Psi$$

$$H_{v}\sum_{k=1}^{N_{b}} x_{k}\Phi_{k} = E\sum_{k=1}^{N_{b}} x_{k}\Phi_{k}$$

$$\times\Phi_{i}^{*} \qquad (i = 1, 2, \cdots, N_{b})$$

$$\sum_{k=1}^{N_{b}} (H_{v})_{ik}x_{k} = Ex_{i}$$

$$\langle\Phi_{i}|\Phi_{k}\rangle = \delta_{ik}$$

Simultaneous Equation

• N_b-dimentional linear simultaneous equations:

$$\begin{pmatrix} (H_v)_{11} & (H_v)_{12} & \cdots & (H_v)_{1N_b} \\ (H_v)_{21} & (H_v)_{22} & \cdots & (H_v)_{2N_b} \\ \vdots & \vdots & \ddots & \vdots \\ (H_v)_{N_b1} & (H_v)_{N_b2} & \cdots & (H_v)_{N_bN_b} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N_b} \end{pmatrix} = E \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N_b} \end{pmatrix}$$

• Diagonalization

 $E = E_1, E_2, \cdots, E_{N_b}$ $\{x\} = x_1, x_2, \cdots, x_{N_b}$

Hamiltonian matrix

 Hamiltonian matrix is decomposed into sub matrices belonging to each value of M



Conservation of M (= Jz) : $M = m_1 + m_2 + \dots + m_k$ [*H*, *J*_z] = 0

What about J?

• An exercise: 2 neutrons in 0f7/2 orbit

J+: Angular momentum raising operator $J_+|J, M\rangle \rightarrow |J, M + 1\rangle$



J = 0 two-body state is lost

J = 1 can be eliminated, but is not contained.

Single-particle orbits



$$NL_{J}$$

$$N = 2n + I (+ 1)$$

$$= 1, 2, 3, ... \qquad J = I + s$$

$$(= 0, 1, 2, ...)$$

Orbital Angular Momentum	Symbol
I = 0	S
l = 1	р
l = 2	d
I = 3	f
I = 4	g
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Figure 2-23 Sequence of one-particle orbits. The figure is taken from M. G. Mayer and J. H. D. Jensen, Elementary Theory of Nuclear Shell Structure, p. 58, Wiley, New York, 1955. m = -7/2, -5/2, ..., 0, 72/2

#(sps) = 2J + 1 = 2x7/2 + 1 = 8

J components in M

2 neutrons in 0f7/2 orbit

	Dimension	J components
M = 0	4	J = 0, 2, 4, 6
M = 1	3	J = 2, 4, 6
M = 2	3	J = 2, 4, 6
M = 3	2	J = 4, 6
M = 4	2	J = 4, 6
M = 5	1	J = 6
M = 6	1	J = 6

M's are conserved w/ the SDs, but J's are mixed for M fixed.

0f7/2

Diagonalization of the Hamiltonian matrix



This property is general, and valid for the cases with more than 2 particles.

Numerical methods of diagonalization

- Algorithm:
- Householder method for smaller matrix-size
- Lanczos method: for larger matrix-size

Traditional diagonalization method

- Lanczos method:
 - Obtain a few eigenvalues from the lowest energy state
 - Start from the initial vector v_1

 $Hv_{1} = \alpha_{1}v_{1} + \beta_{1}v_{2}$ Orthogonalization of Hv_i & v_i, v_{i-1} -> v_{i+1} $Hv_{2} = \beta_{1}v_{1} + \alpha_{2}v_{2} + \beta_{2}v_{3}$ $Hv_{3} = \beta_{2}v_{2} + \alpha_{3}v_{3} + \beta_{3}v_{4}$

Diagonalization of the ith tridiagonal matrix
 Convergence of the eigenvalues, even @ i << n

$$J_i = egin{bmatrix} lpha_1 & eta_1 & & & \ eta_1 & lpha_2 & eta_2 & & & \ & eta_2 & \ddots & & \ & & & eta_2 & \ddots & & \ & & & & eta_{i-1} & eta_{i-1} & \ & & & eta_{i-1} & eta_i \end{bmatrix}$$



Example ($^{18}O = ^{16}O \text{ core} + 2 \text{ n}$)

Shell-model caluculation

- Example: 180 (Z = 8, N = 10)
- Assume 16O (Z = 8, N = 8) as the doubly-closed core
 #(Valence Nucleons): A_v = A A_c = 18 16 = 2
- Take the sd-shell model space



Single-particle energy

• Single-particle energies: taken from the 170 energy spectra

$$H = H_c + H_v = H_c + H_0 + V_v$$

$$H_v = H_0 + V_v$$

$$H_0 \psi_i(\mathbf{r}_j) = \epsilon_i \psi_i(\mathbf{r}_j)$$

Experimentally measured values

$$H_{c} = \sum_{i \leq A_{c}} T_{i} + \sum_{i < j \leq A_{c}} V_{ij} \qquad H_{0} = \sum_{A_{c} < i} (T_{i} + U_{i}) \qquad V_{v} = \sum_{A_{c} < i < j} V_{ij}$$
$$U_{j} = \sum_{i \leq A_{c}} V_{ij}$$
³²

Two-body Matrix Elements

TBME: Phenomenological Effective Interaction

$$H = H_c + H_v = H_c + (H_0 + V_v)$$

 $H_v = H_0 + V_v$

Effective Interaction (determination is explained later)

$$H_{c} = \sum_{i \leq A_{c}} T_{i} + \sum_{i < j \leq A_{c}} V_{ij} \qquad H_{0} = \sum_{A_{c} < i} (T_{i} + U_{i}) \qquad V_{v} = \sum_{A_{c} < i < j} V_{ij}$$
$$U_{j} = \sum_{i \leq A_{c}} V_{ij}$$
33

Basis state

- #(Slater determinant): $\begin{pmatrix} N_{sps} \\ A_v \end{pmatrix} = \frac{12}{2} = 66$
- Conservation of M: $M = m_1 + m_2$
- For M = 0, $N_b = 14$
- Possible M = 0 2-particle states

 $J \ge M$

	(j1 <i>,</i> m1)	(j2, m2)		(j1, m1)	(j2, m2)
1	(5/2, +5/2)	(5/2, -5/2)	8	(5/2, -1/2)	(3/2, +1/2)
2	(5/2, +3/2)	(5/2, -3/2)	9	(5/2, -3/2)	(3/2, +3/2)
3	(5/2, +1/2)	(5/2, -1/2)	10	(1/2, +1/2)	(1/2, -1/2)
4	(5/2, +1/2)	(1/2, -1/2)	11	(1/2, +1/2)	(3/2, -1/2)
5	(5/2, -1/2)	(1/2, +1/2)	12	(1/2, -1/2)	(3/2, +1/2)
6	(5/2, +3/2)	(3/2, -3/2)	13	(3/2, +3/2)	(3/2, -3/2)
7	(5/2, +1/2)	(3/2, -1/2)	14	(3/2, +1/2)	(3/2, -1/2)

180 energy spectra

• Diagonalization of 14x14 Hamiltonian matrix



Some remarks

- 1. TBMEs
- 2. Determination of TBMEs
- 3. Scheme

TBMEs

Two-body matrix elements (TBMEs)

• A two-body state is written as

 $|j_1, j_2, J, M\rangle = \sum_{m_1, m_2} \langle j_1, m_1, j_2, m_2 | J, M \rangle | j_1, m_1 \rangle | j_2, m_2 \rangle$

• Two-body matrix elements (TBMEs)

$$\langle j_1, j_2, J, M | V | j_3, j_4, J', M' \rangle = \sum_{m_1, m_2} \langle j_1, m_1, j_2, m_2 | J, M \rangle \\ \times \sum_{m_1, m_2} \langle j_1, m_1, j_2, m_2 | J', M' \rangle \\ \times \langle j_1, m_1, j_2, m_2 | V | j_3, m_3, j_4, m_4 \rangle | j_2, m_2 \rangle$$

TBMEs can be non-zero, only if J = J' & M = M', because V is rotationally invariant (a scalar w.r.t. the rotation).

$$\left[V,J^2\right] = \left[V,J_z\right] = 0$$
³⁸

Two-body matrix elements (TBMEs)

• Two-body matrix elements (TBMEs)

 $\langle j_1, j_2, J, M | V | j_3, j_4, J, M \rangle$

are independent of M values, also because V is rotationally invariant.

 $\langle j_1, j_2, J | V | j_3, j_4, J \rangle$

$$\left[V,J^2\right] = \left[V,J_z\right] = 0$$

• Two-body matrix elements are assigned by

 j_1, j_2, j_3, j_4 and J

Because of the complexity of nuclear force, one cannot express all TBMEs by few empirical parameters.

Example of the TBMEs

- An example of TBMEs: USD interaction (Wildenthal & Brown)
- Model space: sd-shell (d5/2, d3/2 and s1/2)
- 3 single-particle energies (SPEs): $\epsilon_{0d5/2}$, $\epsilon_{0d3/2}$ and $\epsilon_{1s1/2}$
- **63** TBMEs: $\langle j_1, j_2, J, T | V | j_3, j_4, J, T \rangle$

(Isospin is also a good quantum #)



USD interaction

i	j	k		J	Т	۷
1	1	1	1	0	1	-2.1845
1	1	1	1	1	0	-1.4151
1	1	1	1	2	1	-0.0665
1	1	1	1	3	0	-2.8842
2	1	1	1	1	0	0.5647
2	1	1	1	2	1	-0.6149
2	1	1	1	3	0	2.0337
2	1	2	1	1	0	-6.5058
2	1	2	1	1	1	1.0334
2	1	2	1	2	0	-3.8253
2	1	2	1	2	1	-0.3248
2	1	2	1	3	0	-0.5377
2	1	2	1	3	1	0.5894
2	1	2	1	4	0	-4.5062
2	1	2	1	4	1	-1.4497
2	1	3	1	1	0	-1.7080
2	1	3	1	1	1	0.1874
2	1	3	1	2	0	0.2832
2	1	3	1	2	1	-0.5247
2	1	3	3	1	0	2.1042
2	2	1	1	0	1	-3.1856
2	2	1	1	1	0	0.7221
2	2	1	1	2	1	-1.6221
2	2	1	1	3	0	1.8949
2	2	2	1	1	0	2.5435
2	2	2	1	2	1	-0.2828
2	2	2	1	3	0	2.2216
2	2	2	1	4	1	-1.2363
2	2	2	2	0	1	-2.8197
2	2	2	2	1	0	-1.6321
2	2	2	2	2	1	-1.0020
2	2	2	2	3	0	-1.5012

•

•

i,j,k,l 1: 0d3/2 2: 0d5/2 3: 1s1/2

Dimensions

- Dimension: Maximum # of the basis
- sd-shell: 8 < (Z, N) < 20 ((sd)ⁿ configuration)
- pf-shell: 20 < (Z, N) < 40 ((pf)ⁿ configuration)





Determination of the TBMEs

Shell-Model Hamiltonian



Determination of the TBMEs

- Early time: Closed shell + Experimental levels of 2 valence particles
 TBME
- Example: 0⁺, 2⁺, 4⁺, 6⁺ in ⁴²Ca: well isolated 0f7/2 orbit



$$V_{J} = \langle 0f7/2, 0f7/2, J, T = 1 | V | 0f7/2, 0f7/2, J, T = 1 \rangle$$

are determined directly by the experimental observations.

Experimental energy of state J \downarrow $E(J) = 2 \epsilon(0f7/2) + V_J$ Experimental single-particle energy of 0f7/2

Single-particle orbits



$$NL_{J}$$

$$N = 2n + I (+ 1)$$

$$= 1, 2, 3, ... \qquad J = I + s$$

$$(= 0, 1, 2, ...)$$

Orbital Angular Momentum	Symbol
I = 0	S
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Figure 2-23 Sequence of one-particle orbits. The figure is taken from M. G. Mayer and J. H. D. Jensen, Elementary Theory of Nuclear Shell Structure, p. 58, Wiley, New York, 1955. m = -7/2, -5/2, ..., 0, 74/2

#(sps) = 2J + 1 = 2x7/2 + 1 = 8

Empirical determination

- The isolation of 0f7/2 is special. In the other cases, several orbits must be taken into account.
- In general, chi² fit is made as follows,

(1) TBMEs are assumed.

(2) chi² fit is calculated btw theor. & exp. energy levels.

(3) TBMEs are modified.

(4) Go to (1), & iterate (1)-(3) until chi² becomes small enough

• Example: 0⁺, 2⁺, 4⁺ in ¹⁸O: 0d5/2 & 1s1/2

 $\langle 0d5/2, 0d5/2, J, T = 1 | V | 0d5/2, 0d5/2, J, T = 1 \rangle$ $\langle 0d5/2, 1s1/2, J, T = 1 | V | 0d5/2, 0s1/2, J, T = 1 \rangle$.

Arima, Cohen, Lawson & McFarlane (1968)

- At the beginning, it was a perfect chi² fit.
- As heavier nuclei are studied,

(1) the number of TBMEs increases,

(2) shell-model calculations become huge



Hybrid version

Hybrid version

• Microscopically calculated TBMEs eg.) G-matrix (Kuo-Brown, H.-Jensen, ...)

G-matrix based TBMEs are not perfecxt direct use for shell model calculation is only disaster

 Use G-matrix-based TBMEs as a starting point of the chi^2 fit, and do the chi^2 fit to the experiments.
 (Consider some linear combinations of TBMEs and fit them)

cont'd

- The chi² fit method produces, as a result of minimization, a set of linear equations of TBMEs
- Some linear combinations of TBMEs are sensitive to available experimental data (ground & low-lying states).

The others are insensitive. Those are assumed to be given by G-matrixbased calculation (i.e. no fit).

Firstly done for sd-shell: Wildenthal & Brown's USD interaction
 47 linear combinations (1970)

Recent version of USD: G-matrix-based TBMEs have been improved -> 30 linear combinations fitted

Example

• An example from pf-shell (f7/2, f5/2, p3/2, p1/2)

<u>G-matrix + polarization correction + empirical refinement</u> Microscopic Empirical (Phenomenological)

- GXPF1 interaction: M. Honma et al., PRC65 (2002) 061301(R)
- start from a realistic microscopic interaction
- M. Hjorth-Jensen, et al., Phys. Rept. 261 (1995) 125
 - Bonn-C potential
 - 3rd order Q-box + folded diagram
- ✓ 195 TBMEs & 4 SPEs are calculated -> not completely good (theory imperfect)
- Vary 70 linear combinations of 195 TBME2 & 4 SPEs
- ➢ Fit to 699 exp. energy data of 87 nuclei

Single-particle orbits



Figure 2-23 Sequence of one-particle orbits. The figure is taken from M. G. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure*, p. 58, Wiley, New York, 1955.

G-matrix vs. GXPF1A



Scheme

Prescriptions of Shell-model calc.

- M-scheme
 - basis function: Slater determinant
 - SD does not hold J as a good quantum #, but eigen function after the diagonalization holds J as a good quantum #.

$$\left[H_v, J^2\right] = \left[H_v, J_z\right] = 0$$

• J-scheme

- basis function: $\Phi_{JM} = \sum_{m_1,m_2} \langle j_1 m_1 j_2 m_2 | JM \rangle \psi_{j_1 m_1} \psi_{j_2 m_2}$ $\begin{bmatrix} H, J^2 \end{bmatrix} = 0$

- JT-scheme $\left[H, T^2\right] = 0$
- M-scheme + J-projection
- ...

J-scheme



Configuration	J = 0	J = 1	J = 2	J = 3	J = 4
(d5/2) ²	\checkmark		\checkmark		\checkmark
(d5/2)(s1/2)			\checkmark	\checkmark	
(s1/2) ²	\checkmark				
(d5/2)(d3/2)		\checkmark	\checkmark	\checkmark	\checkmark
(s1/2)(d3/2)		\checkmark	\checkmark		
(d3/2) ²	\checkmark		\checkmark		

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1	(5/2, +5/2)	(5/2, -5/2)	8	(5/2, -1/2)	(3/2, +1/2)
2	(5/2, +3/2)	(5/2, -3/2)	9	(5/2, -3/2)	(3/2, +3/2)
3	(5/2, +1/2)	(5/2, -1/2)	10	(1/2, +1/2)	(1/2, -1/2)
4	(5/2, +1/2)	(1/2, -1/2)	11	(1/2, +1/2)	(3/2, -1/2)
5	(5/2, -1/2)	(1/2, +1/2)	12	(1/2, -1/2)	(3/2, +1/2)
6	(5/2, +3/2)	(3/2, -3/2)	13	(3/2, +3/2)	(3/2, -3/2)
7	(5/2, +1/2)	(3/2, -1/2)	14	(3/2, +1/2)	(3/2, -1/2)

Summary



Slide from M. Honma



- f5pg9-殻 JUN45相互作用
 - 137パラメータ中45線形結合を 400データにフィット
 - 平均誤差185keV
 - g9/2軌道(異パリティ)の影響
- sd-pf 殻
 - ⁴⁰Ca閉殻の構造
 - 重いsd 設中性子過剰核
- - N=Z近傍核の陽子過剰核
 - 変形共存と形状相転移
 - 重いpf 設中性子過剰核
 - ¹⁰⁰Snの閉殻構造



End