

- 日本物理学会第63回年次大会講演 2008/3/26aZH-10 於近畿大学

スピン軌道力を取り入れた 正準基底HFB法プログラムの開発

*Development of a canonical-basis HFB program
including spin-orbit force*

(1) Formulation

特に(昨秋の学会講演の補足として)準粒子ハミルトニアンに対角化法

(2) Si アイソトープの計算結果

田嶋直樹 (福井大工)

Naoki Tajima, Fukui University

URL http://www.apphy.fukui-u.ac.jp/~tajima/jpsm07fl_slide.pdf (昨秋分)
[jpsm08sp_slide.pdf](http://www.apphy.fukui-u.ac.jp/~tajima/jpsm08sp_slide.pdf) (公開予定)

正準基底HFB法とは

正準基底HFB法

未知の核 ⇒ 任意の変形、任意の表面状態 (スキン、ハロー)
調和振動子等の基底展開は不利 (最適化がわずらわしい)
位置座標表現が適する (正方メッシュ表現等)

中性子過剰核 ⇒ フェルミ準位の上昇 (連続状態への接近)
対相関で連続状態を陽に取り入れる必要
位置座標表現で従来の解法 (準粒子法)は困難 (状態数が過大)

正準基底HFB法 + 3次元メッシュ表現 + Skyrme 相互作用
任意の変形、任意の表面状態、連続状態の対相関 を扱える

HFB in canonical-basis method

HFB solutions can be expressed in the **BCS form**

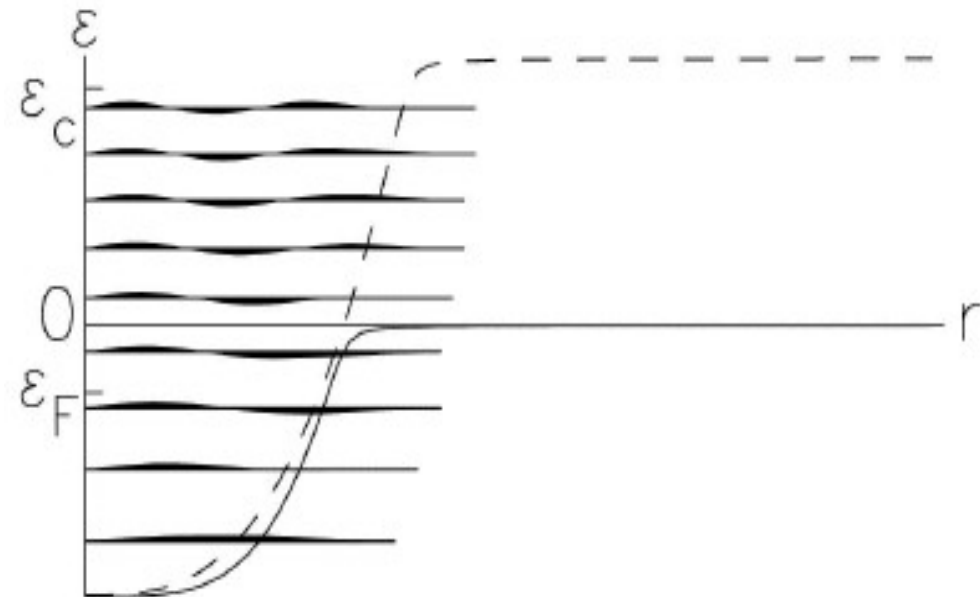
$$|\Psi\rangle = \prod_{i=1}^{i_{\max}} (u_i + v_i a_i^\dagger a_i^\dagger) |0\rangle$$

$$a_i^\dagger = \sum_s \int d^3r \psi_i(\vec{r}, s) a^\dagger(\vec{r}, s) \quad : \text{HFB canonical basis}$$

$$\frac{\delta E}{\delta \psi_i^*} = \mathcal{H}_i \psi_i = \sum_j \lambda_{ij} \psi_j, \quad \mathcal{H}_i = v_i^2 h + u_i v_i \tilde{h}$$

h : Hartree-Fock Hamiltonian

\tilde{h} : Pairing Hamiltonian



HFB CANONICAL BASIS

Skyrme HFB法におけるスピン軌道力

Ref. Bonche et al., Nucl.Phys. A443, 39 (1985)

HFB with the Skyrme force

Mean-field interaction:

$$\hat{v} = t_0(1 + x_0 P_\sigma)\delta + \frac{1}{2}t_1(1 + x_1 P_\sigma)(\vec{k}^2\delta + \delta\vec{k}^2) + t_2(1 + x_2 P_\sigma)\vec{k} \cdot \delta\vec{k} \\ + \frac{1}{6}\rho^\alpha t_3(1 + x_3 P_\sigma)\delta + iW(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k} \times \delta\vec{k}$$

Pairing interaction: different parameters assumed, only for (S=0, T=1) pairs.

$$\hat{v}_p = v_p \frac{1 - P_\sigma}{2} \left\{ \left[1 - \frac{\rho}{\rho_c} - \frac{\rho_n - \rho_p}{\rho'_c} T_z - \left(\frac{\tilde{\rho}}{\tilde{\rho}_c} \right)^2 \right] \delta - \frac{1}{2k_c^2} (\vec{k}^2\delta + \delta\vec{k}^2) \right\}$$

- v_p : overall strength, to be adjusted depending on the cutoff.

Cutoff can also be controlled by the number of canonical basis.

- $\rho_c = 0.32 \text{ fm}^{-3}$, $\rho'_c = \tilde{\rho}_c = \infty$: density dependence, insufficient information
- $k_c = 2 \text{ fm}^{-1}$: momentum dependence (=finite range effect), prevents the point collapse

See http://www.apphy.fukui-u.ac.jp/~tajima/jpsm07fl_slide.pdf for details.

時間反転対称性の利用

Time reversal symmetry

The time-reversal operator T can be defined in $|\vec{r}s\rangle$ representation by

$$T|\uparrow\rangle = |\downarrow\rangle, \quad T|\downarrow\rangle = -|\uparrow\rangle, \quad T\psi(\vec{r}) = \psi^*(\vec{r})T$$

Thus, for

$$|\psi\rangle = \int d^3r [\psi_{\uparrow}(\vec{r}) |\vec{r}\uparrow\rangle + \psi_{\downarrow}(\vec{r}) |\vec{r}\downarrow\rangle],$$

$$|\bar{\psi}\rangle = T|\psi\rangle = \int d^3r [\psi_{\uparrow}^*(\vec{r}) |\vec{r}\downarrow\rangle - \psi_{\downarrow}^*(\vec{r}) |\vec{r}\uparrow\rangle].$$

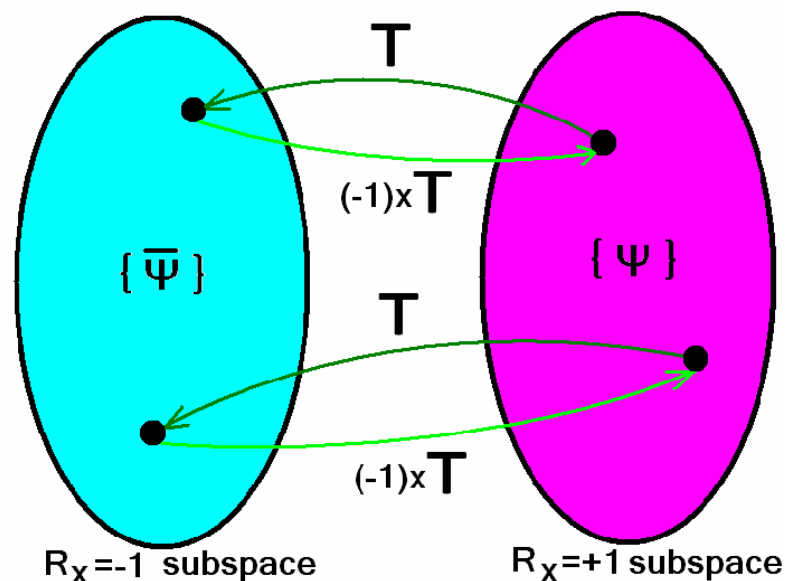
We use four real-value functions of \vec{r} , $\{ \psi^{(1)}(\vec{r}), \psi^{(2)}(\vec{r}), \psi^{(3)}(\vec{r}), \psi^{(4)}(\vec{r}) \}$, to express a time-reversal pair of orbitals.

$$\psi(\vec{r}, s) = \left[\psi^{(1)}(\vec{r}) + i\psi^{(2)}(\vec{r}) \right] \delta_{s\uparrow} + \left[\psi^{(3)}(\vec{r}) + i\psi^{(4)}(\vec{r}) \right] \delta_{s\downarrow},$$

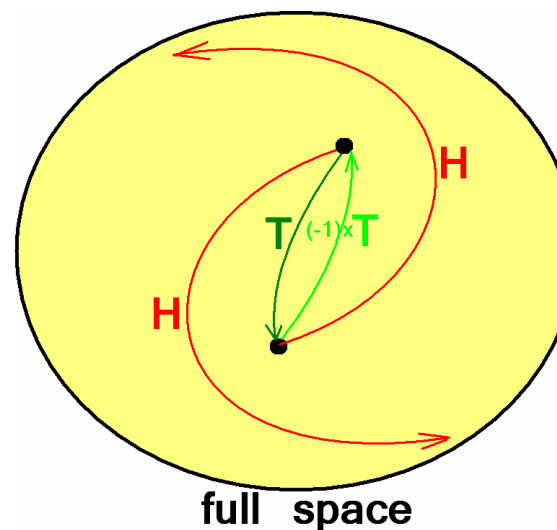
$$\bar{\psi}(\vec{r}, s) = \left[-\psi^{(3)}(\vec{r}) + i\psi^{(4)}(\vec{r}) \right] \delta_{s\uparrow} + \left[\psi^{(1)}(\vec{r}) - i\psi^{(2)}(\vec{r}) \right] \delta_{s\downarrow},$$

Time reversal and spatial symmetries

- In other works, spatial symmetries are imposed (e.g., D_{2h} , C_4 , C_{1h} , R_1), under which time reversal partners can be assigned to different subspaces.



- On the other hand, in this work, we do not impose any spatial symmetries and thus it is not possible to prefix a subspace for $i > 0$ or $i < 0$.



準粒子ハミルトニアンに対角化法

Gradient step evolution で正準基底を改良していくと同時に、200 stepsくらいに1回の頻度でよいので、その時点の正準基底の張る部分空間内で、その時点の準粒子ハミルトニアンを対角し、得られた準粒子によりHFB解の一体密度を作り、その一体密度の固有状態としてよりよい正準基底を得ることで収束を早めることができる。

Diagonalization of HFB quasiparticle Hamiltonian in the subspace spanned by the canonical basis

For $|\alpha\rangle, |\beta\rangle \in \{|1\rangle, \dots, |M\rangle, |\bar{1}\rangle, \dots, |\bar{M}\rangle\}$

h : mean-field Hamiltonian

\tilde{h} : pairing Hamiltonian

$$h^\dagger = h, \quad [T, h] = 0$$

$$\tilde{h}^\dagger = \tilde{h}, \quad [T, \tilde{h}] = 0$$

$$H_{\alpha\beta} = \langle \alpha | (h - \epsilon_F) | \beta \rangle$$

$$\Delta_{\alpha\beta} = \langle \alpha | \tilde{h}T | \beta \rangle$$

for $1 \leq i, j \leq M$

$$\begin{cases} A_{ij} = \langle i | (h - \epsilon_F) | j \rangle \\ B_{ij} = \langle \bar{i} | (h - \epsilon_F) | j \rangle \end{cases}$$

for $1 \leq i, j \leq M$

$$\begin{cases} C_{ij} = \langle i | \tilde{h} | j \rangle \\ D_{ij} = \langle \bar{i} | \tilde{h} | j \rangle \end{cases}$$

$$H = \begin{pmatrix} A & -B^* \\ B & A^* \end{pmatrix}$$

$$\Delta = \begin{pmatrix} -D^* & -C \\ C^* & -D \end{pmatrix}$$

$$A^\dagger = A, \quad B^T = -B, \quad H^\dagger = H$$

$$C^\dagger = C, \quad D^T = -D, \quad \Delta^\dagger = \Delta$$

Quasiparticle Hamiltonian is defined in the doubled basis
 $\{ |1\rangle, \dots, |M\rangle, |\bar{1}\rangle, \dots, |\bar{M}\rangle, |1\rangle, \dots, |M\rangle, |\bar{1}\rangle, \dots, |\bar{M}\rangle \}$

$$\mathcal{H} = \begin{pmatrix} H & \Delta \\ -\Delta^* & -H^* \end{pmatrix} \quad (\mathcal{H}^\dagger = \mathcal{H})$$

For $\epsilon_\alpha > 0$ ($\alpha = 1, \dots, 2M$), **quasiparticle states** are

$$\mathcal{H} \begin{pmatrix} U_\alpha \\ V_\alpha \end{pmatrix} = \epsilon_\alpha \begin{pmatrix} U_\alpha \\ V_\alpha \end{pmatrix}, \quad \mathcal{H} \begin{pmatrix} V_\alpha^* \\ U_\alpha^* \end{pmatrix} = -\epsilon_\alpha \begin{pmatrix} V_\alpha^* \\ U_\alpha^* \end{pmatrix}.$$

V_α : spatially localized

U_α : spatially localized for $0 < \epsilon_\alpha < -\epsilon_F$, dislocalized for $\epsilon_\alpha > -\epsilon_F$

All the above calculations are to obtain the one-body density :

$$\rho = V^* V^T, \quad V = (V_1, \dots, V_{2M})$$

The one-body density ρ is very useful because

the eigenstates of ρ are an improved set of canonical basis states.

It guides the gradient step evolution to a fast convergence path.

note 1) One expects to obtain the eigenstates pairwise.

$$\begin{aligned}\rho W_i &= v_i^2 W_i, & |i\rangle' &= \sum_{j=1}^M (W_{ji} |j\rangle + W_{\bar{j}i} |\bar{j}\rangle), \\ \rho W_{\bar{i}} &= v_{\bar{i}}^2 W_{\bar{i}}, & |\bar{i}\rangle' &= \sum_{j=1}^M (W_{j\bar{i}} |j\rangle + W_{\bar{j}\bar{i}} |\bar{j}\rangle).\end{aligned}$$

It must hold $W_{j\bar{i}} = -W_{\bar{j}i}^*$, $W_{\bar{j}\bar{i}} = W_{ji}^*$.

No numerical troubles encountered.

note 2) One has to adjust the Fermi level ϵ_f to fulfill $N = \text{Tr}\rho$ and thus one has to repeat the above procedure many times.

Si同位体の計算結果

Test calculation

Nucleus: $Z = 14$, $6 \leq N \leq 34$

Mean field:

Skyrme SIII force, including the **spin-orbit** force,
but excluding the Coulomb force

Pairing force:

$$k_c = 2 \text{ fm}^{-1}, \rho_c = 0.32 \text{ fm}^{-3}, v_p = -1050 \text{ MeV fm}^3$$

The number of the canonical basis states:

three times as many as the number of neutrons/protons (N=14)

$$2M = N + 2 \cdot 14^{2/3} N^{1/3}$$

Box: Cube with edge $L = 25.6 \text{ fm} \rightarrow 40 \text{ fm} \rightarrow 60.8 \text{ fm}$,
(31^3 points $\rightarrow 49^3$ points $\rightarrow 75^3$ points)

mesh spacing $\Delta x = 0.8 \text{ fm}$

Initial state: Harmonic oscillator state with $\beta_2 = 0.3$, $\gamma = 30^\circ$.

The number of canonical basis states

An estimation in terms of a harmonic oscillator relation

$$\Gamma(N_{\text{osc}}) \doteq \frac{1}{3}(N_{\text{osc}} + 2)^3 : \text{主量子数 } N_{\text{osc}} \text{ 以下の状態数 (近似式)}$$

(1) energy up to the Fermi level + ϵ_{cut}

$$2M = \frac{N}{3} \left\{ 3^{1/3} + 2^{1/3} \frac{\epsilon_{\text{cut}}}{(41 \text{ MeV})} \right\}^3$$

$$= \begin{cases} 2N & \text{for } \epsilon_{\text{cut}} = 12\text{MeV} \text{ 「2倍スペース」} \\ 3N & \text{for } \epsilon_{\text{cut}} = 21\text{MeV} \text{ 「3倍スペース」} \\ 4N & \text{for } \epsilon_{\text{cut}} = 28\text{MeV} \text{ 「4倍スペース」} \end{cases}$$

\Rightarrow Empirically, pairing gap is roughly independent of N .

(2) n -major shells above the Fermi level ($\epsilon_{\text{cut}} = 41nA^{-1/3}$ MeV, $A = 2N$)

$$2M = N \left\{ 1 + \frac{n}{(3N)^{1/3}} \right\}^3 = N + 3^{2/3} n N^{2/3} + \dots$$

\Rightarrow Dependence on N is still too weak.

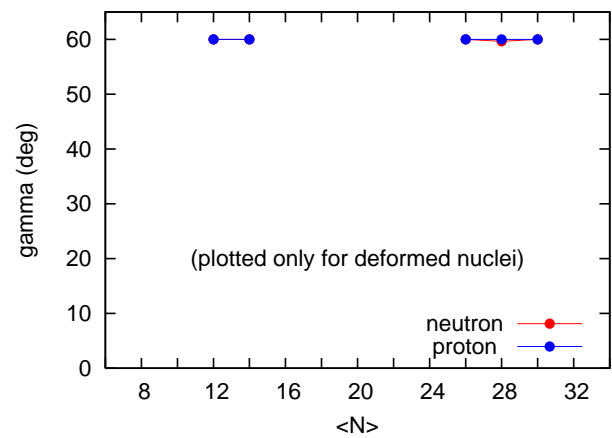
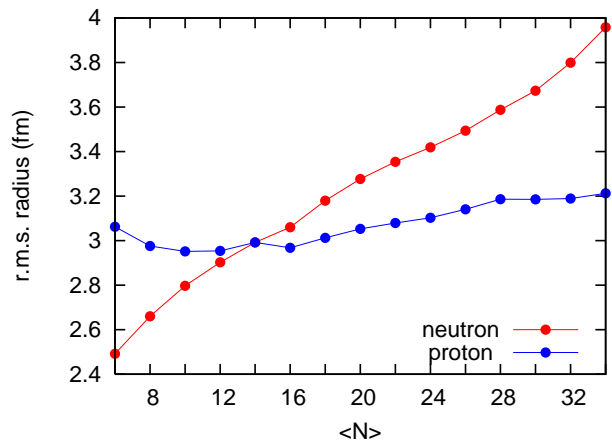
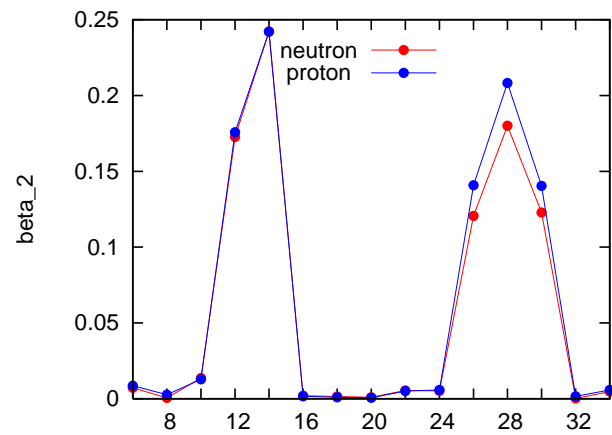
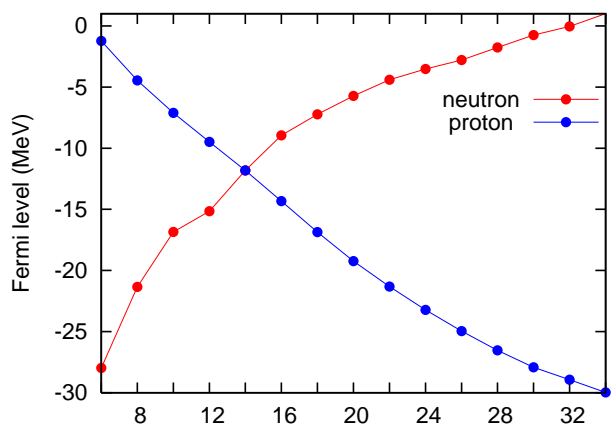
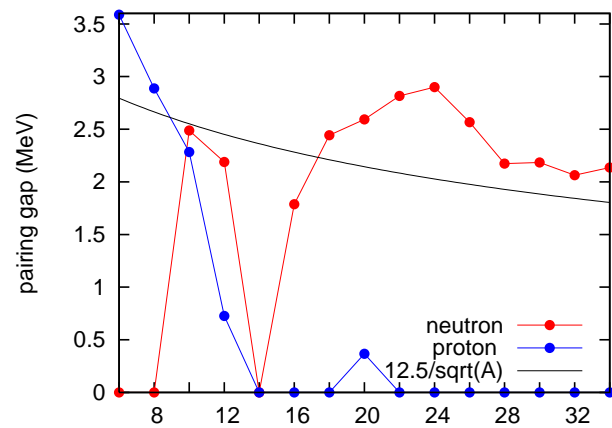
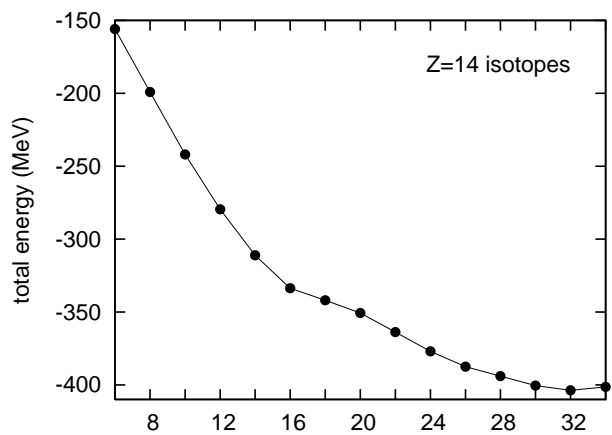
(3) In this talk, I choose

for $Z = 14$ isotopes, $2M = N + 2 \cdot 14^{2/3} N^{1/3}$

($N = Z = 14$ で3倍スペース, $1.5\hbar\omega$ カットオフ)

for $N = Z = 150$, $2M = 150$

(2倍スペース)



解の精度

HFB 解では

$$H_i |i\rangle = \sum_{j=1}^{2M} |j\rangle \langle j| H_i |i\rangle$$

が成立. そこで

$$|R_i\rangle = H_i |i\rangle - \sum_{j=1}^{2M} |j\rangle \langle j| H_i |i\rangle$$

として

$$\Delta\epsilon_i := \langle R_i | R_i \rangle$$

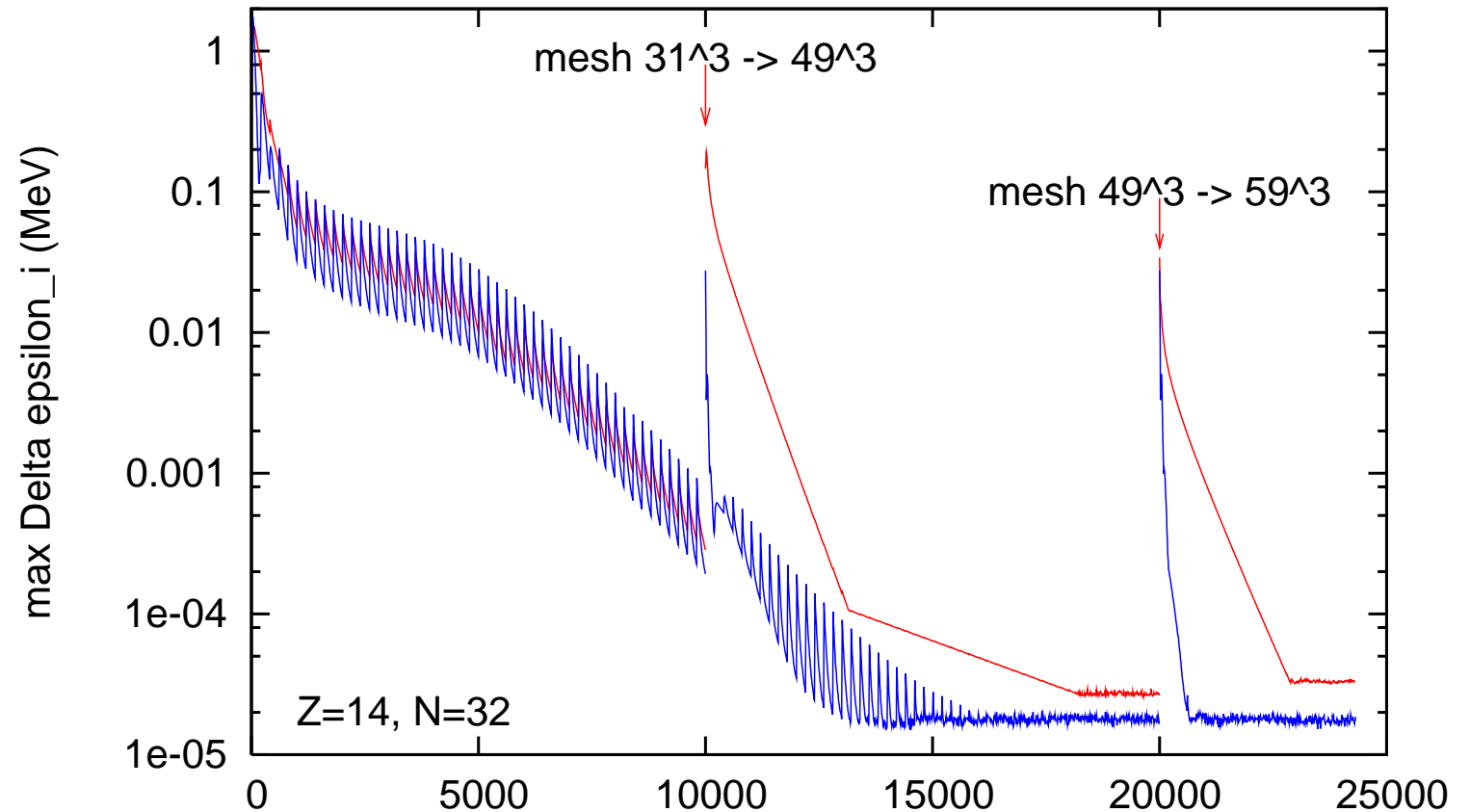
$$= \langle i | H_i^2 |i\rangle - \sum_{j=1}^{2M} |\langle j | H_i |i\rangle|^2$$

と定義される量が

解の精度の目安となる.

ただし正規直交時に

ゼロとなる項は省いた.



青線：陽子、赤線：中性子

$Z=14, N=32$ (a nucleus in the drip line)

Neutron's Fermi level = -40 keV

By changing the length of the box edge

$L = 25.6\text{fm} \rightarrow 40\text{fm}$

$$|\Delta E| = -50 \text{ keV}$$

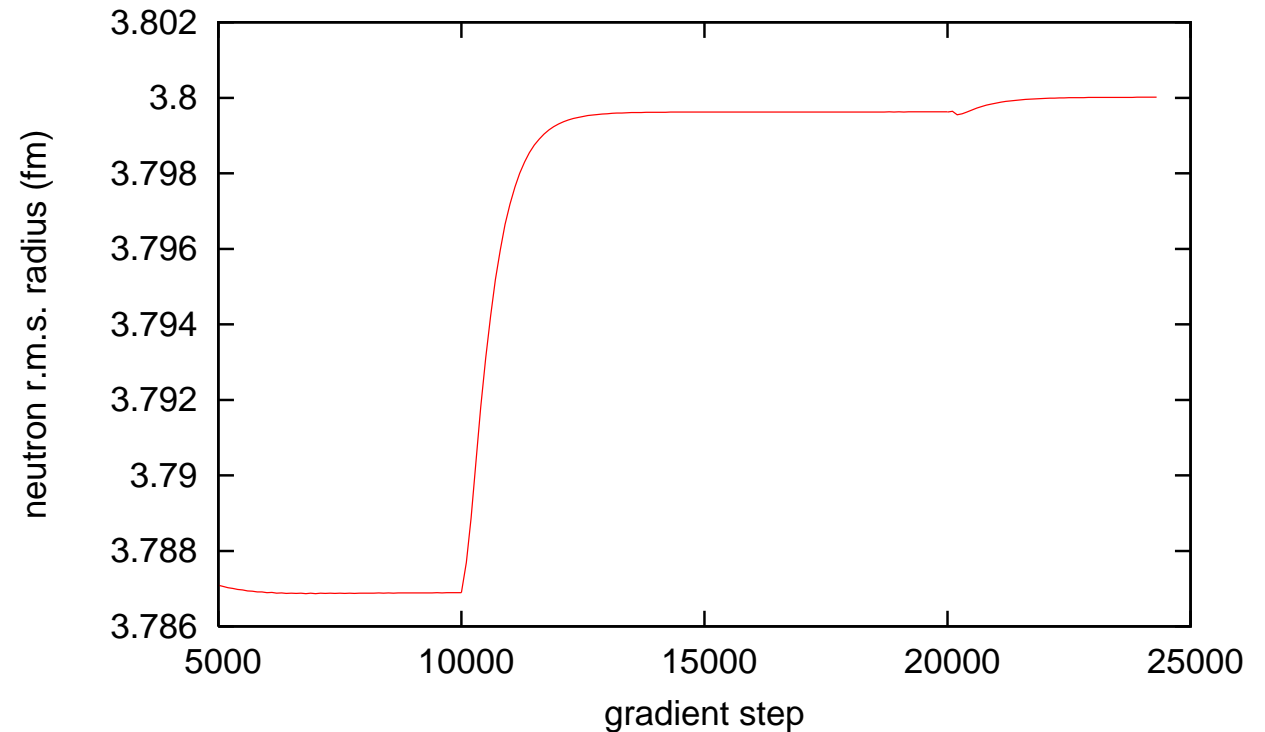
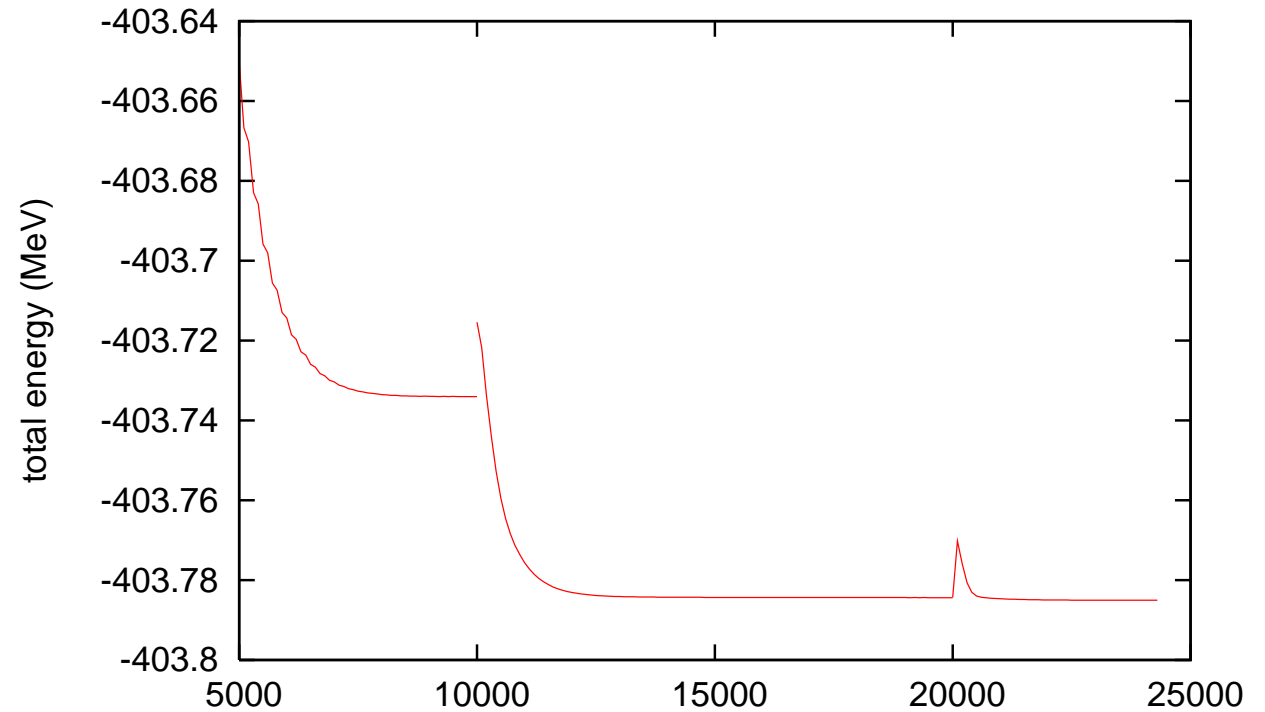
$$\Delta r_{\text{rms}} = 0.013 \text{ fm}$$

$L=40\text{fm} \rightarrow 60.8\text{fm}$

$$|\Delta E| < 1 \text{ keV}$$

$$\Delta r_{\text{rms}} = 0.0003 \text{ fm}$$

Even for this extremely weakly bound nucleus, there is no difficulty to expand the box size until the result converges.



まとめ

1. 正準基底HFB法プログラムを、**スピン軌道力**が扱えるように改造した。
2. 空間的対称性を一切課さず、一方、**時間反転対称性**は最大限に利用した。
3. $Z=14$ 同位体の計算例を示した。**ドリップ線**まで何の困難もなく扱えた。
4. 昨秋、計算途中まで示した $N=Z=150$ 核の計算についても、対角化時の問題を解消でき、**超重核**でも扱える計算法であることが確かめられた。ただし、計算時間不足で完全には収束していないため今回はグラフを示さなかった。

今後の計画

1. **クーロンポテンシャル**の導入 → 完了後、論文としてまとめる。
2. プログラムの活用、対相関の反中性子暈効果の系統的研究、**核図表**全面の計算。
3. 各種の**拘束項**の導入、外場による変形の収束の加速。