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対相関の中性子暈抑制効果と核変形II

Pairing anti-neutron-halo effect and nuclear deformation II

(1) スピン軌道力を取り入れるための正準基底HFB法の改造

(2) テスト計算結果の1例

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前回までの講演の要点

今春の物理学会での中性子暈についての報告内容

球形核では

対相関がなければ、
対相関があれば、

束縛の減少につれ平均半径が漸増
pairing anti-halo effect

変形核では

対相関の有無によらず、

フェルミ準位の上昇による平均半径の増加率は小さい

変形核でも球形核でも

対相関がなければ、

フェルミ準位がゼロを超えれば、HF解は密度が非局在化する。

対相関があれば、

フェルミ準位がゼロを超えても、

しばらくは密度の局在したHFB解が存続する。

⇒ドリップ線だからと言って粒子数射影が

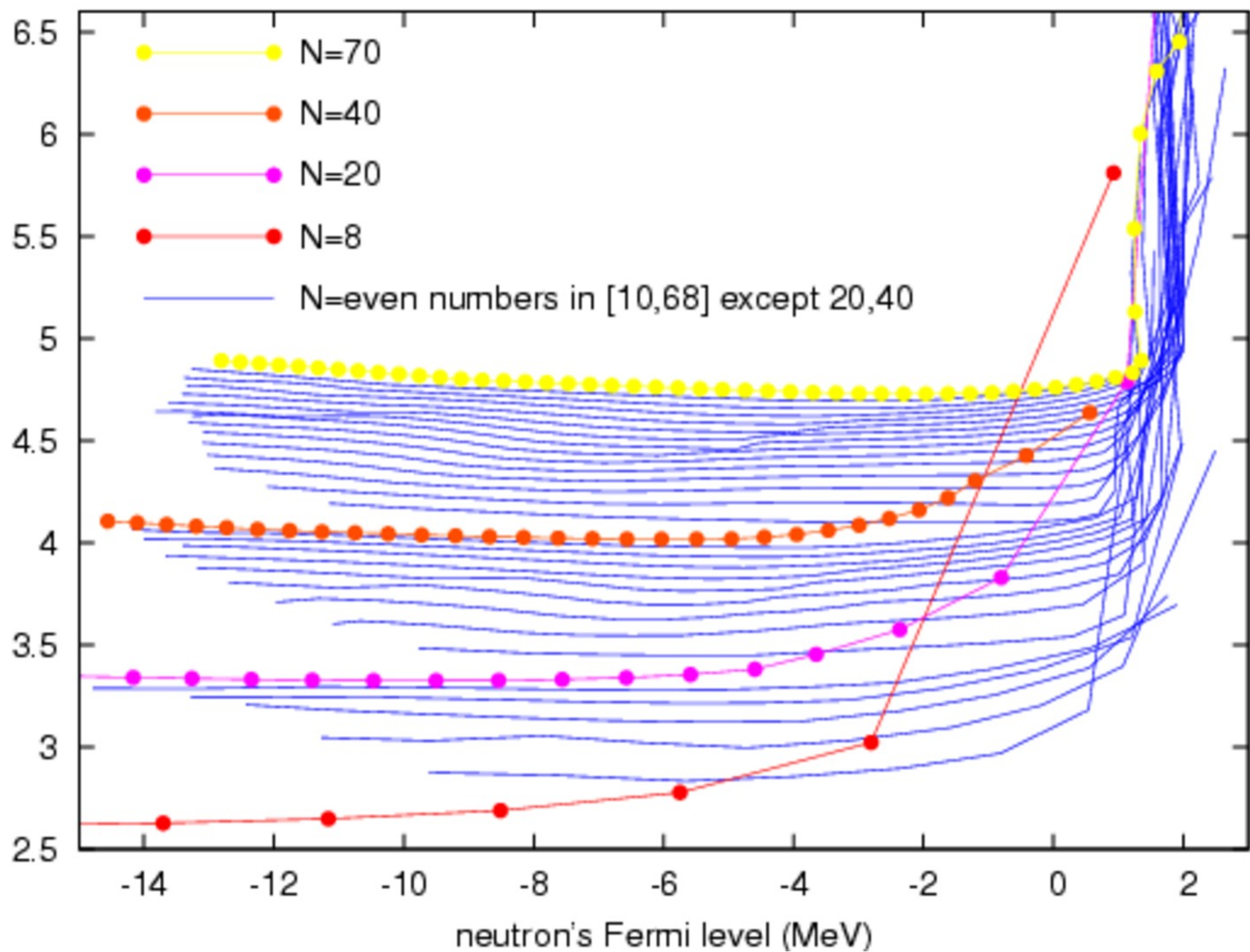
特に必要になる訳ではない。

今回は、講演「part II」としてスピン軌道を入れた計算を示したかったが...

⇒ スピン軌道を導入し終えたところで時間切れ。

テスト計算結果を1例だけ示す。

neutron's r.m.s. radius (fm)



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
従来の解法 (準粒子法) では困難 (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**

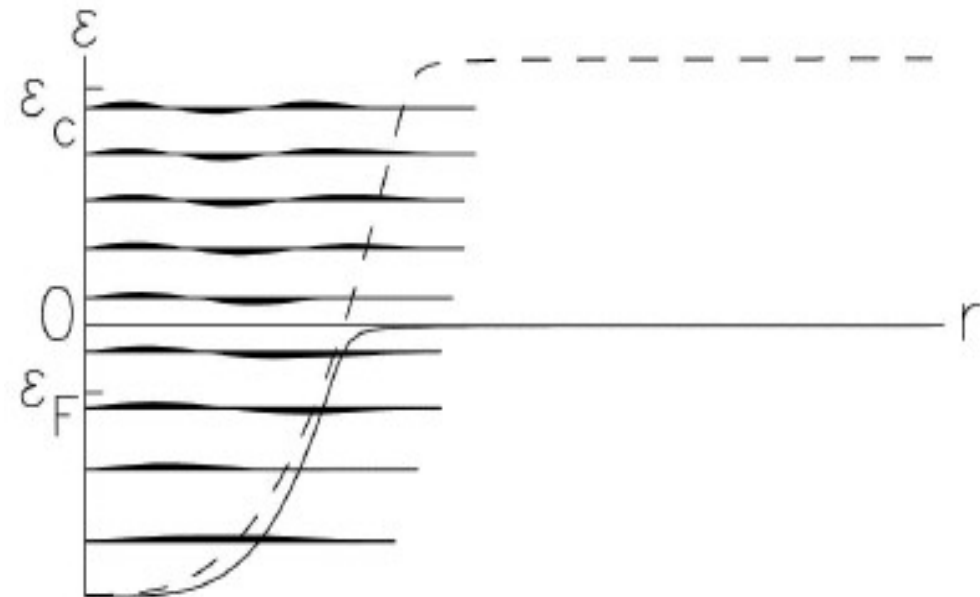
$$|\Psi\rangle = \prod_{i=1}^{i_{\max}} (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger) |0\rangle$$

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

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

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)

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.

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

Hamiltonian density for even-even nuclei

$$\begin{aligned}
 E = \int \mathcal{H} d\vec{r}, \quad \mathcal{H} = & \frac{\hbar^2}{2m} (\tau_n + \tau_p) \\
 & + C_1 (\rho_n^2 + \rho_p^2) + C'_1 \rho_n \rho_p \\
 & + C_2 (\rho_n \tau_n + \rho_p \tau_p) + C'_2 (\rho_n \tau_p + \rho_p \tau_n) \\
 & + C_3 (\rho_n \vec{\nabla}^2 \rho_n + \rho_p \vec{\nabla}^2 \rho_p) + C'_3 (\rho_n \vec{\nabla}^2 \rho_p + \rho_p \vec{\nabla}^2 \rho_n) \\
 & + C_4 \rho^\alpha (\rho_n^2 + \rho_p^2) + C'_4 \rho^\alpha \rho_n \rho_p \\
 & + C_5 (\rho_n \vec{\nabla} \cdot \vec{J}_n + \rho_p \vec{\nabla} \cdot \vec{J}_p) + C'_5 (\rho_n \vec{\nabla} \cdot \vec{J}_p + \rho_p \vec{\nabla} \cdot \vec{J}_n) \\
 & + C_6 \tilde{\rho}_n^2 + C_7 \rho_n \tilde{\rho}_n^2 + C'_7 \rho_p \tilde{\rho}_n^2 + C_8 \tilde{\rho}_n^4 + C_9 \tilde{\rho}_n (\tilde{\tau}_n - \vec{\nabla}^2 \tilde{\rho}_n) \\
 & + C_6 \tilde{\rho}_p^2 + C_7 \rho_p \tilde{\rho}_p^2 + C'_7 \rho_n \tilde{\rho}_p^2 + C_8 \tilde{\rho}_p^4 + C_9 \tilde{\rho}_p (\tilde{\tau}_p - \vec{\nabla}^2 \tilde{\rho}_p) \\
 & + C_{10} V_C \rho_p + C_{11} \rho_p^{4/3}
 \end{aligned}$$

where

$$\begin{aligned}
 C_1 &= \frac{1}{4} t_0 (1 - x_0) & C'_1 &= \frac{1}{2} t_0 (2 + x_0) \\
 C_2 &= \frac{1}{8} (t_1 (1 - x_1) + 3t_2 (1 + x_2)) & C'_2 &= \frac{1}{8} (t_1 (2 + x_1) + t_2 (2 + x_2)) \\
 C_3 &= \frac{3}{32} (t_1 (x_1 - 1) + t_2 (x_2 + 1)) & C'_3 &= \frac{1}{32} (-3t_1 (2 + x_1) + t_2 (2 + x_2)) \\
 C_4 &= \frac{1}{24} t_3 (1 - x_3) & C'_4 &= \frac{1}{12} t_3 (2 + x_3) \\
 C_5 &= -W & C'_5 &= -\frac{1}{2} W \\
 C_6 &= \frac{1}{4} v_P & & \\
 C_7 &= -\frac{1}{4} v_P \left(\frac{1}{\rho_c} + \frac{1}{\rho'_c} \right) & C'_7 &= -\frac{1}{4} v_P \left(\frac{1}{\rho_c} - \frac{1}{\rho'_c} \right) \\
 C_8 &= -\frac{1}{4} \frac{v_P}{\tilde{\rho}_c^2} & C_9 &= -\frac{1}{4} \frac{v_P}{k_c^2} \\
 C_{10} &= \frac{1}{2} & C_{11} &= -\frac{3}{4} e^2 \left(\frac{3}{\pi} \right)^{1/3}
 \end{aligned}$$

Densities ($\mathbf{q} = \mathbf{n}, \mathbf{p}$)

$$\begin{aligned}\tau_{\mathbf{q}}(\vec{r}) &= 2 \sum_{s=\uparrow\downarrow} \sum_{i>0} v_{qi}^2 |\vec{\nabla} \psi_{qi}(\vec{r}, s)|^2, & \tilde{\tau}_{\mathbf{q}}(\vec{r}) &= 2 \sum_{s=\uparrow\downarrow} \sum_{i>0} u_{qi} v_{qi} |\vec{\nabla} \psi_{qi}(\vec{r}, s)|^2, \\ \rho_{\mathbf{q}}(\vec{r}) &= 2 \sum_{s=\uparrow\downarrow} \sum_{i>0} v_{qi}^2 |\psi_{qi}(\vec{r}, s)|^2, & \tilde{\rho}_{\mathbf{q}}(\vec{r}) &= 2 \sum_{s=\uparrow\downarrow} \sum_{i>0} u_{qi} v_{qi} |\psi_{qi}(\vec{r}, s)|^2,\end{aligned}$$

$$\vec{\nabla} \cdot \vec{J}_{\mathbf{q}}(\vec{r}) = \frac{2}{i} \sum_{s'=\uparrow\downarrow} \sum_{s=\uparrow\downarrow} \sum_{i>0} v_{qi}^2 \left[\vec{\nabla} \psi_{qi}^*(\vec{r}, s') \right] \times \left[\vec{\nabla} \psi_{qi}(\vec{r}, s) \right] \cdot \vec{\sigma}_{s's}.$$

State dependent Hamiltonian : $\mathcal{H}_{qi} \psi_{qi} = \delta E / \delta \psi_{qi}^*$

$$\begin{aligned}h_{\mathbf{q}} &= -\vec{\nabla} \cdot B_{\mathbf{q}} \vec{\nabla} + V_{\mathbf{q}} + i \vec{W}_{\mathbf{q}} \cdot \vec{\sigma} \times \vec{\nabla} & : \text{mean-field Hamiltonian} \\ \tilde{h}_{\mathbf{q}} &= -\vec{\nabla} \cdot \tilde{B}_{\mathbf{q}} \vec{\nabla} + \tilde{V}_{\mathbf{q}} & : \text{pairing Hamiltonian} \\ \mathcal{H}_{qi} &= v_{qi}^2 h_{\mathbf{q}} + u_{qi} v_{qi} \tilde{h}_{\mathbf{q}} & : \text{Hamiltonian of } i\text{th canonical orbital}\end{aligned}$$

Effective masses and single-particle potentials

$$\begin{aligned}B_{\mathbf{n}} &= \frac{\hbar^2}{2m} + C_2 \rho_{\mathbf{n}} + C'_2 \rho_{\mathbf{p}} \\ \tilde{B}_{\mathbf{n}} &= C_9 \tilde{\rho}_{\mathbf{n}} \\ V_{\mathbf{n}} &= 2C_1 \rho_{\mathbf{n}} + C'_1 \rho_{\mathbf{p}} + C_2 \tau_{\mathbf{n}} + C'_2 \tau_{\mathbf{p}} + 2C_3 \vec{\nabla}^2 \rho_{\mathbf{n}} + 2C'_3 \vec{\nabla}^2 \rho_{\mathbf{p}} \\ &\quad + \rho^{\alpha-1} \left[(\alpha+2) C_4 \rho_{\mathbf{n}}^2 + (\alpha C_4 + C'_4) \rho_{\mathbf{p}}^2 + (2C_4 + (\alpha+1) C'_4) \rho_{\mathbf{n}} \rho_{\mathbf{p}} \right] \\ &\quad + C_5 \vec{\nabla} \cdot \vec{J}_{\mathbf{n}} + C'_5 \vec{\nabla} \cdot \vec{J}_{\mathbf{p}} + C_7 \tilde{\rho}_{\mathbf{n}}^2 + C'_7 \tilde{\rho}_{\mathbf{p}}^2 \\ \vec{W}_{\mathbf{n}} &= -C_5 \vec{\nabla} \rho_{\mathbf{n}} - C'_5 \vec{\nabla} \rho_{\mathbf{p}} \\ \tilde{V}_{\mathbf{n}} &= 2C_6 \tilde{\rho}_{\mathbf{n}} + 2C_7 \rho_{\mathbf{n}} \tilde{\rho}_{\mathbf{n}} + 2C'_7 \rho_{\mathbf{p}} \tilde{\rho}_{\mathbf{n}} + 4C_8 \tilde{\rho}_{\mathbf{n}}^3 + C_9 \left(\tilde{\tau}_{\mathbf{n}} - 2\vec{\nabla}^2 \tilde{\rho}_{\mathbf{n}} \right)\end{aligned}$$

Operation of the spin-orbit potential to a set of four real wavefunctions

$$|\psi'\rangle = i\vec{W} \cdot \vec{\sigma} \times \vec{\nabla} |\psi\rangle$$

By expressing ψ in terms of a set of four real wavefunctions as
 $\psi(\vec{r}, s) = [\psi^{(1)}(\vec{r}) + i\psi^{(2)}(\vec{r})] \delta_{s\uparrow} + [\psi^{(3)}(\vec{r}) + i\psi^{(4)}(\vec{r})] \delta_{s\downarrow}$,

$$\begin{pmatrix} \psi'^{(1)} \\ \psi'^{(2)} \\ \psi'^{(3)} \\ \psi'^{(4)} \end{pmatrix} = \left(W_x \frac{\partial}{\partial y} - W_y \frac{\partial}{\partial x} \right) \begin{pmatrix} \psi^{(2)} \\ -\psi^{(1)} \\ -\psi^{(4)} \\ \psi^{(3)} \end{pmatrix} + \left(W_y \frac{\partial}{\partial z} - W_z \frac{\partial}{\partial y} \right) \begin{pmatrix} \psi^{(4)} \\ -\psi^{(3)} \\ \psi^{(2)} \\ -\psi^{(1)} \end{pmatrix} + \left(W_z \frac{\partial}{\partial x} - W_x \frac{\partial}{\partial z} \right) \begin{pmatrix} -\psi^{(3)} \\ -\psi^{(4)} \\ \psi^{(1)} \\ \psi^{(2)} \end{pmatrix}$$

- Only through the spin-orbit potential, the four components $\psi^{(1)}, \dots, \psi^{(4)}$ mix with each other. Without the spin-orbit potential, one needs only one real wavefunction with the spin state factorized.
- This mixing is local, while numerical differentiations are very nonlocal. The latter has to be paid much more attention in programming. Thus, four real components are better than two complex components.

Divergence of the spin-orbit current

$$\vec{J}(\vec{r}) = i \sum_{s'=\uparrow\downarrow} \sum_{s=\uparrow\downarrow} \sum_{i>0} 2v_i^2 \psi_i^*(\vec{r}, s') \vec{\sigma}_{s's} \times \vec{\nabla} \psi_i(\vec{r}, s)$$

$$\vec{\nabla} \cdot \vec{J}(\vec{r}) = i \sum_{s'=\uparrow\downarrow} \sum_{s=\uparrow\downarrow} \sum_{i>0} 2v_i^2 \left[\vec{\nabla} \psi_i^*(\vec{r}, s') \right] \cdot \vec{\sigma}_{s's} \times \left[\vec{\nabla} \psi_i(\vec{r}, s) \right]$$

By expressing ψ_i with the four real functions of \vec{r} , $\{\psi_i^{(1)}, \psi_i^{(2)}, \psi_i^{(3)}, \psi_i^{(4)}\}$,

$$\vec{\nabla} \cdot \vec{J} = \sum_{i>0} 4v_i^2 \left\{ \begin{aligned} & \left(\frac{\partial}{\partial x} \psi_i^{(1)} \right) \left(\frac{\partial}{\partial y} \psi_i^{(2)} \right) - \left(\frac{\partial}{\partial x} \psi_i^{(2)} \right) \left(\frac{\partial}{\partial y} \psi_i^{(1)} \right) - \left(\frac{\partial}{\partial x} \psi_i^{(3)} \right) \left(\frac{\partial}{\partial y} \psi_i^{(4)} \right) + \left(\frac{\partial}{\partial x} \psi_i^{(4)} \right) \left(\frac{\partial}{\partial y} \psi_i^{(3)} \right) \\ & + \left(\frac{\partial}{\partial y} \psi_i^{(1)} \right) \left(\frac{\partial}{\partial z} \psi_i^{(4)} \right) - \left(\frac{\partial}{\partial y} \psi_i^{(2)} \right) \left(\frac{\partial}{\partial z} \psi_i^{(3)} \right) + \left(\frac{\partial}{\partial y} \psi_i^{(3)} \right) \left(\frac{\partial}{\partial z} \psi_i^{(2)} \right) - \left(\frac{\partial}{\partial y} \psi_i^{(4)} \right) \left(\frac{\partial}{\partial z} \psi_i^{(1)} \right) \\ & - \left(\frac{\partial}{\partial z} \psi_i^{(1)} \right) \left(\frac{\partial}{\partial x} \psi_i^{(3)} \right) - \left(\frac{\partial}{\partial z} \psi_i^{(2)} \right) \left(\frac{\partial}{\partial x} \psi_i^{(4)} \right) + \left(\frac{\partial}{\partial z} \psi_i^{(3)} \right) \left(\frac{\partial}{\partial x} \psi_i^{(1)} \right) + \left(\frac{\partial}{\partial z} \psi_i^{(4)} \right) \left(\frac{\partial}{\partial x} \psi_i^{(2)} \right) \end{aligned} \right\}$$

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.

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

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

Evolution of a time reversal pair of wavefunctions

- $\langle \bar{\psi} | \psi \rangle = 0$
- $H | \bar{\psi} \rangle = \overline{H | \psi \rangle}$

A gradient-method (imaginary time evolution) step under the orthogonality condition for a pair of wavefunctions

$$\Delta | \psi_i \rangle = -\alpha_i \Delta t \left[\mathcal{H}_i | \psi_i \rangle - \sum_{j>0} (\lambda_{ij} | \psi_j \rangle + \lambda_{i\bar{j}} | \psi_{\bar{j}} \rangle) \right],$$

$$\Delta | \psi_{\bar{i}} \rangle = -\alpha_{\bar{i}} \Delta t \left[\mathcal{H}_{\bar{i}} | \psi_{\bar{i}} \rangle - \sum_{j>0} (\lambda_{\bar{i}j} | \psi_j \rangle + \lambda_{\bar{i}\bar{j}} | \psi_{\bar{j}} \rangle) \right],$$

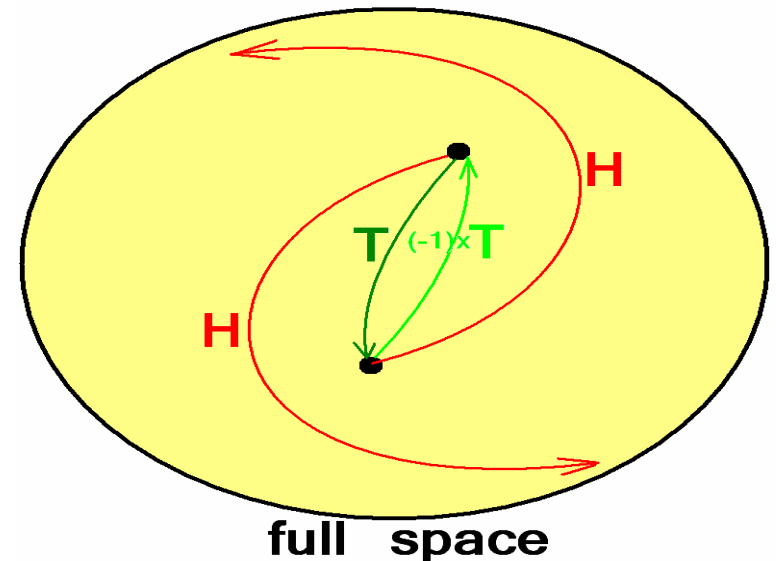
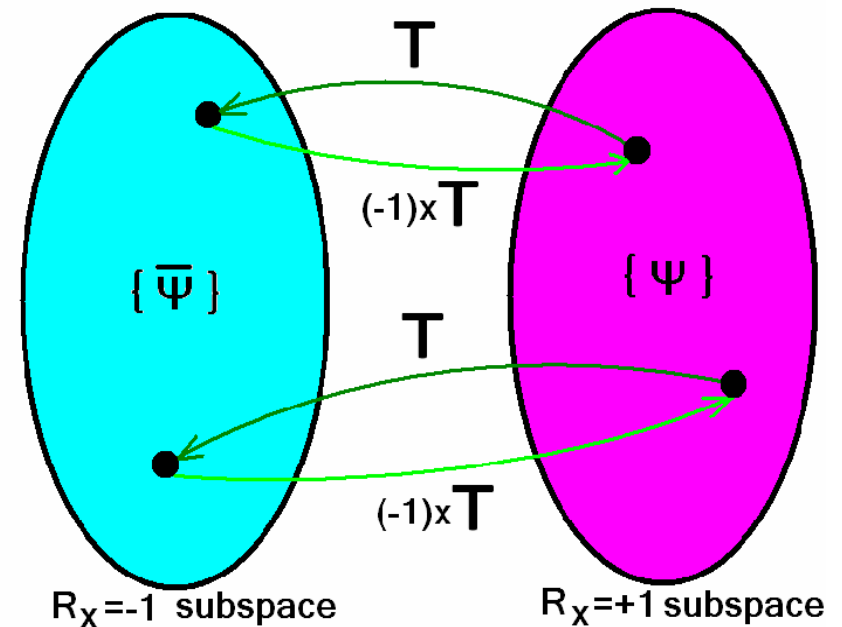
with $\lambda_{\mu\nu} = \frac{1}{\alpha_\mu + \alpha_\nu} \langle \psi_\nu | \alpha_\mu \mathcal{H}_\mu + \alpha_\nu \mathcal{H}_\nu | \psi_\mu \rangle$, $\mathcal{H}_{-\mu} = \mathcal{H}_\mu$, $\alpha_{-\mu} = \alpha_\mu$,

- $\Delta | \psi_{\bar{i}} \rangle = \overline{\Delta | \psi_i \rangle}$

The above evolution rule can be conveniently expressed as that for $\{ \psi_i^{(1)}, \psi_i^{(2)}, \psi_i^{(3)}, \psi_i^{(4)} \}$.

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 $i < 0$.



テスト計算の結果

A test calculation

Nucleus: $N = Z = 150$

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:

twice as many as the number of neutrons/protons

Time-reversal symmetry is maximally utilized.

Box: Cube with edge $L = 32 \text{ fm}$, mesh spacing $\Delta x = 0.8 \text{ fm}$

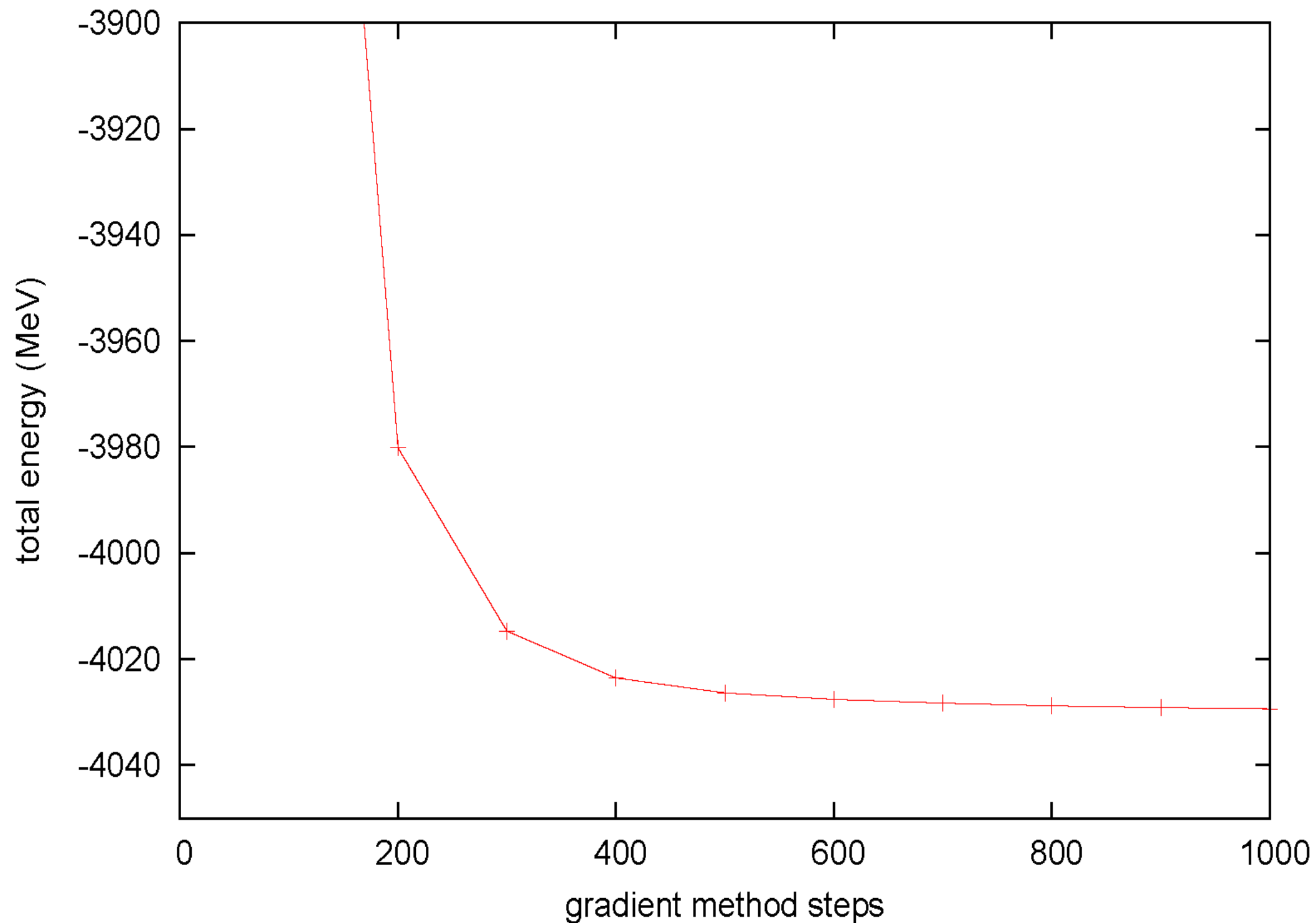
Compared with calculations without the spin-orbit force,

- memory : $\times 4$
- computing time : $\times 6$

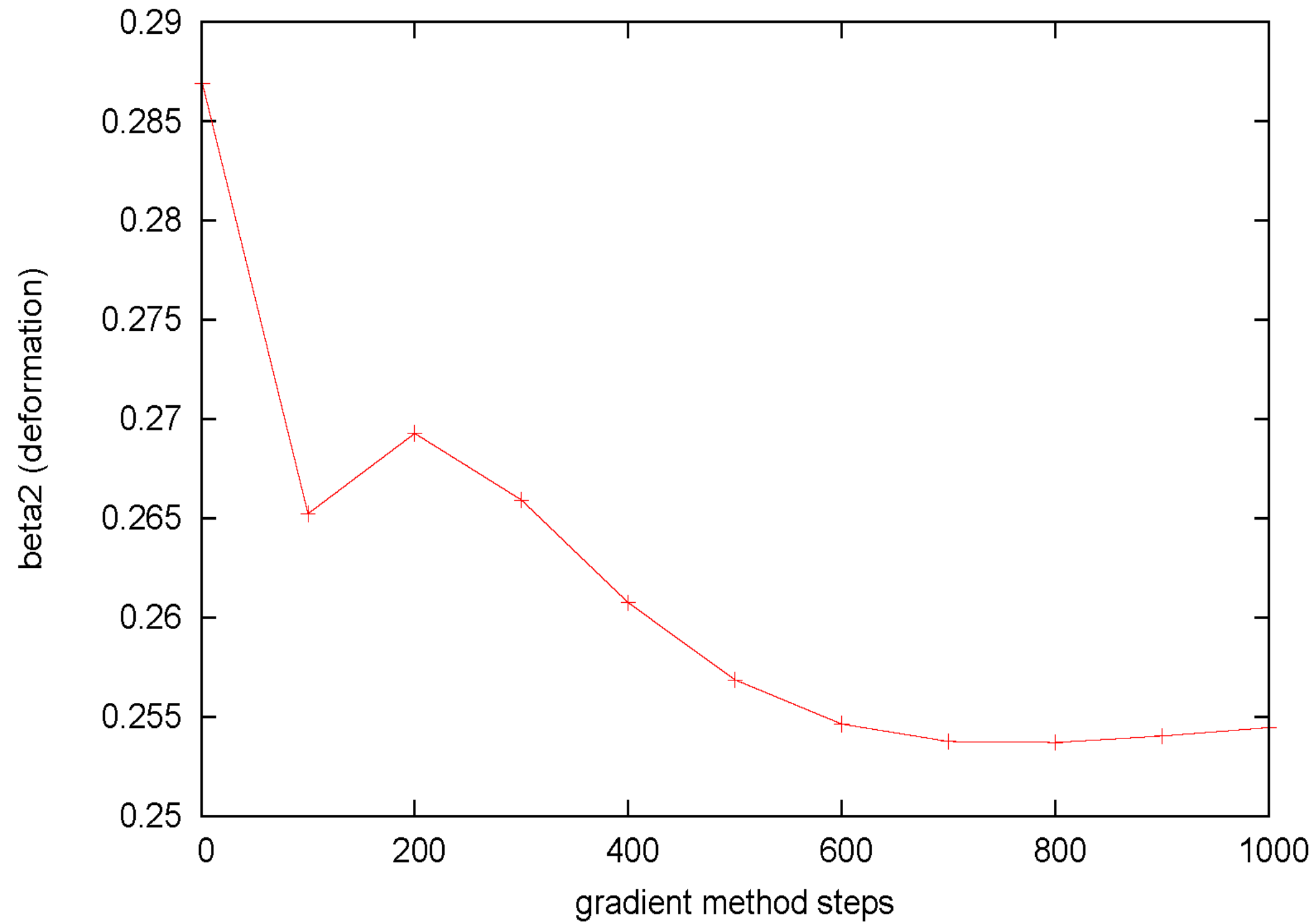
Compared with single-core CPU one-type-of-nucleon calculations,

- dual-core CPU neutron/proton parallel computing time : $\times 1.2$

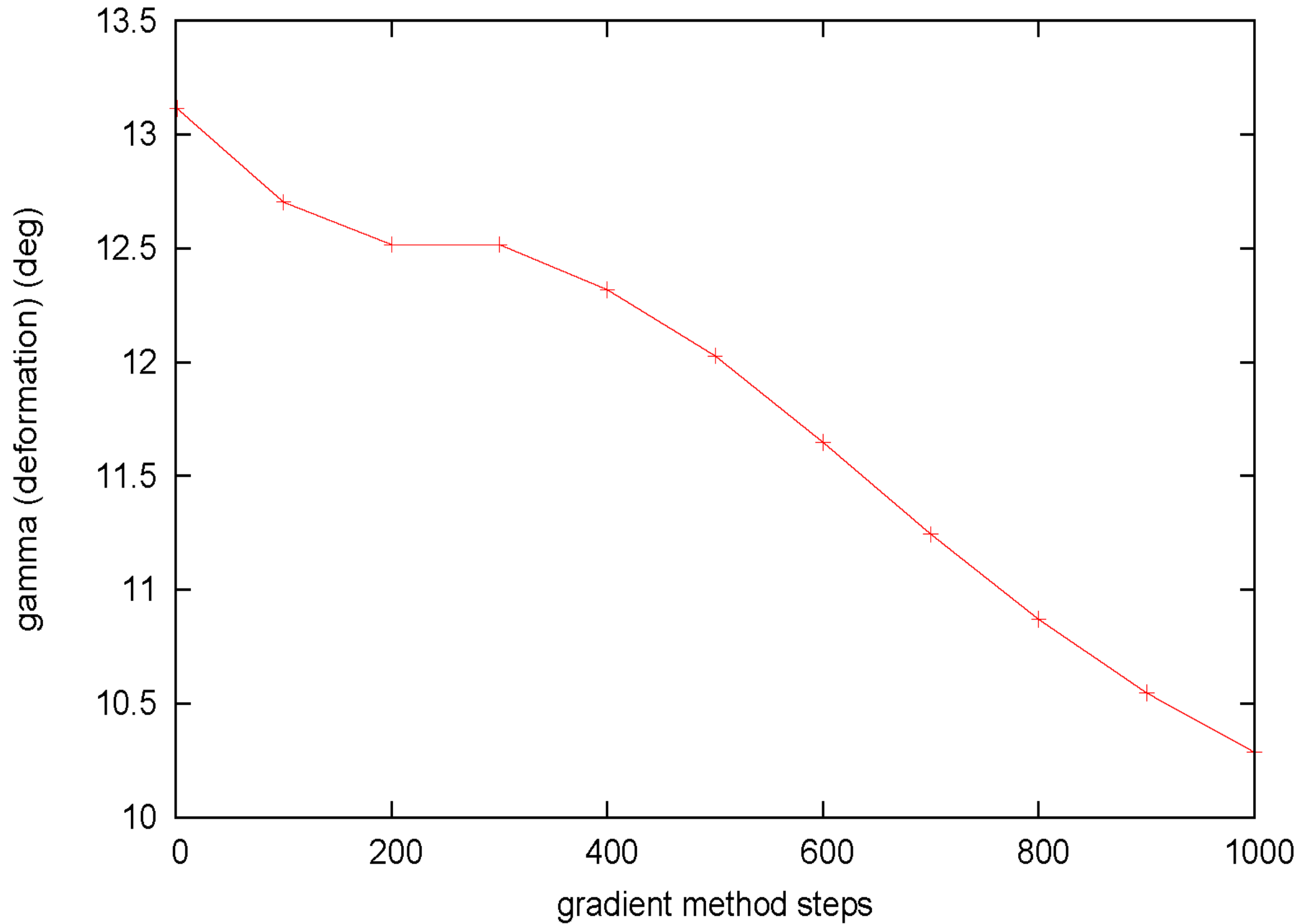
N=Z=150, x2 canonical basis, SIII force, w/o Coulomb



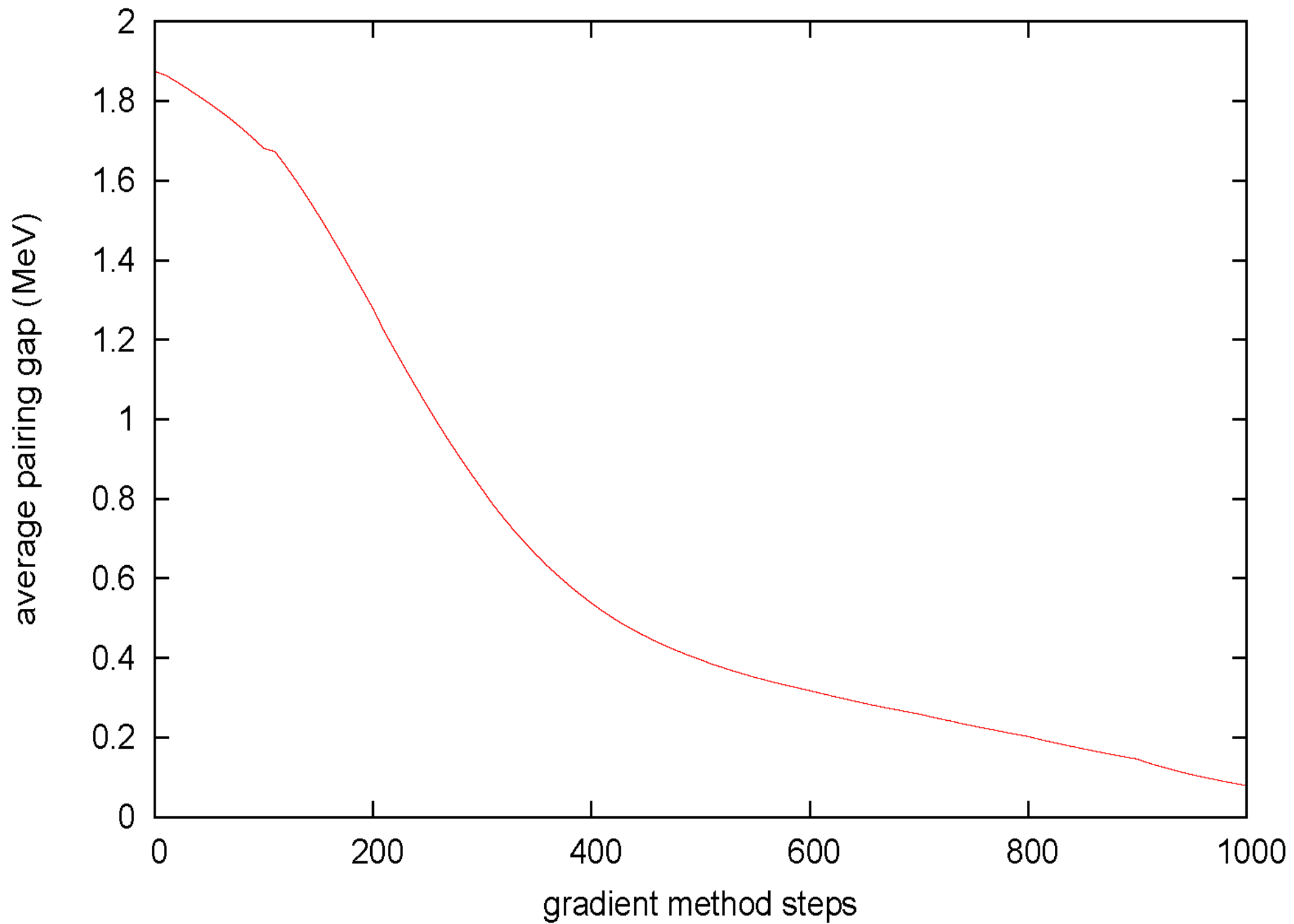
N=Z=150, x2 canonical basis, SIII force, w/o Coulomb



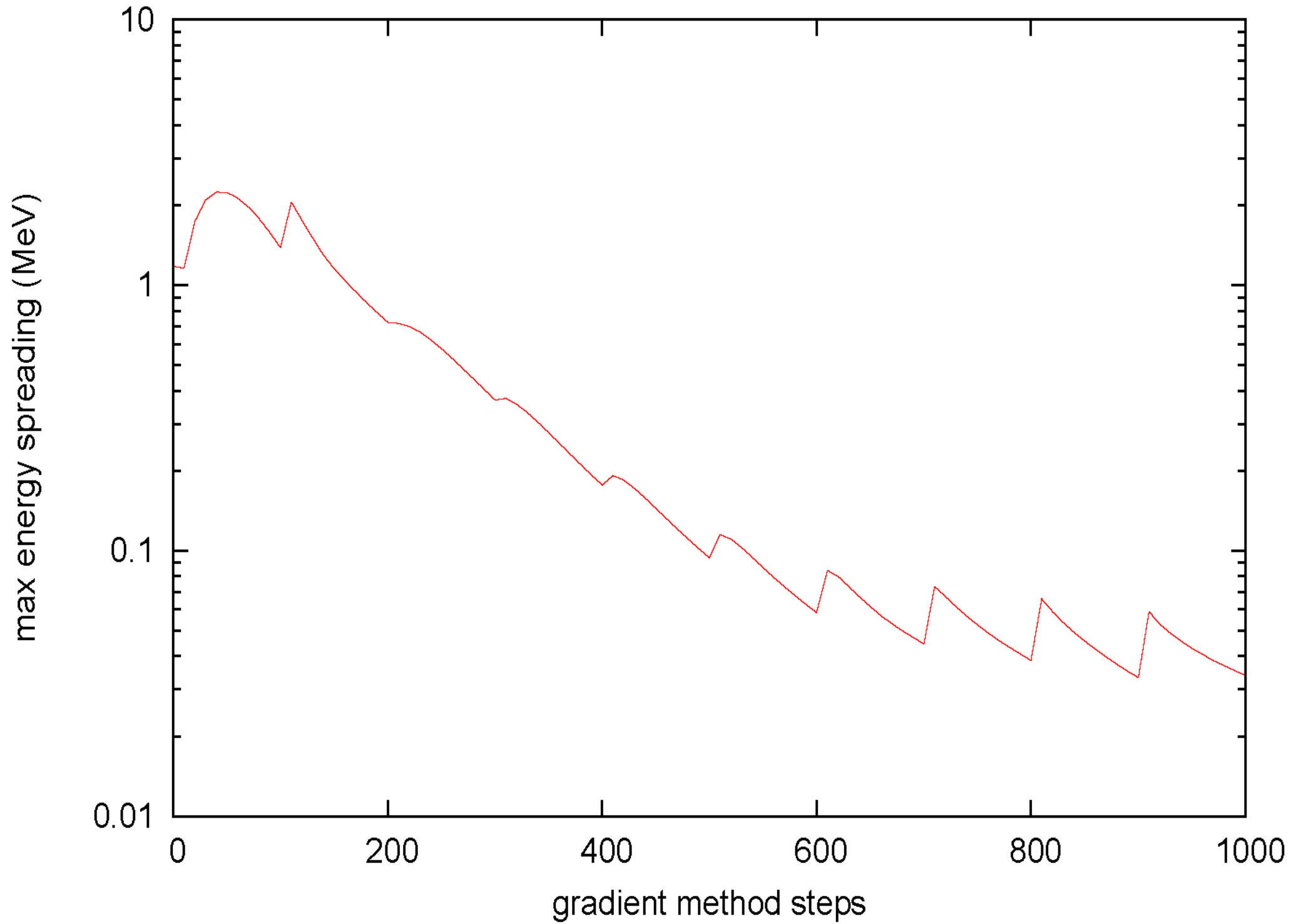
N=Z=150, x2 canonical basis, SIII force, w/o Coulomb



N=Z=150, x2 canonical basis, SIII force, w/o Coulomb



N=Z=150, x2 canonical basis, SIII force, w/o Coulomb



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. $N=Z=150$ 核の基底状態の計算例を示した。
スピン軌道力の導入による計算時間の増加は6倍程度で済んだ。

今後の計画

1. プログラムの気になる点の詰め、 計算効率の向上
2. クーロンポテンシャルの導入、 境界条件の計算方法の選択が重要
3. プログラムの精密な検証
4. 各種の拘束項の導入、 特に回転・並進運動の抑止がたぶん必要となるだろう
変形に対してソフトな核では収束の加速のための外場が必要だろう
5. 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