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Canonical-basis HFB method

— drip lines and beyond —

Naoki Tajima, Fukui University

Contents

1. A new method to obtain the solutions of the HFB equation directory in its canonical form
   - advantages and disadvantages
   - practical and conceptual significance

2. Extension of the code to the full Skyrme energy density functional
   - is uder way. A new progress is an extension to $N \neq Z$ nuclei.
   - Spin-orbit and Coulomb forces are not considered.

3. Calculation of the isotope chain of $_{14}$Si
   - reaching the neutron drip line
   - beyond the neutron drip line

4. Summary

To treat the neutron-rich side of the nuclear chart, one has to take into accout

1. Pairing in the continuum

$$\epsilon_{\rm F} > -\tfrac{1}{2}\hbar\omega_{\rm osc} \text{ (at least half of the shell needed)} \quad \longrightarrow \quad \frac{10^4}{2} \text{ nuclides}$$

2. Long tail for large r $\quad \epsilon_{\rm F} > -1$ MeV $\quad$ for halo

$$\rho(r) \sim \left(\frac{e^{-\kappa r}}{r}\right)^2, \qquad \kappa = \frac{\sqrt{-2m\epsilon_{\rm F}}}{\hbar}$$

pairing $\longrightarrow$ shorter tail

$$\epsilon_{\rm F} \longrightarrow \epsilon_{\rm F} - E_{\rm qp}^{(\rm min)} \quad \text{(deepened)}, \quad E_{\rm qp}^{(\rm min)} \sim \Delta\text{(pairing gap)}$$

3. Deformation $\quad$ all but near spherical magics

$\Rightarrow$ **Coordinate-space Hartree-Fock-Bogoliubov method**

such as 3D Cartesian mesh
feasible for Skyrme force

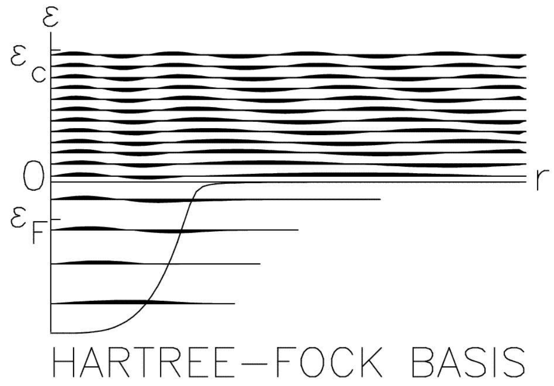
not HF+BCS

$\Rightarrow$ Now there is a new method to solve it : **the Canonical-basis HFB method** !

HFB in quasi-particle method

$$|\psi\rangle = \prod_{i=1}^{\#\text{basis}} b_i|0\rangle$$
$$b_i = \sum_s \int d^3r \left\{\phi_i^*(\vec{r},s)\ a(\vec{r},s) + \psi_i(\vec{r},s)\ a^\dagger(\vec{r},s)\right\}$$

$$\begin{pmatrix} -h & \tilde{h} \\ \tilde{h} & h \end{pmatrix}\begin{pmatrix} \phi_i \\ \psi_i \end{pmatrix} = \epsilon_i \begin{pmatrix} \phi_i \\ \psi_i \end{pmatrix}$$



(≈ QUASI–PARTICLE STATES)

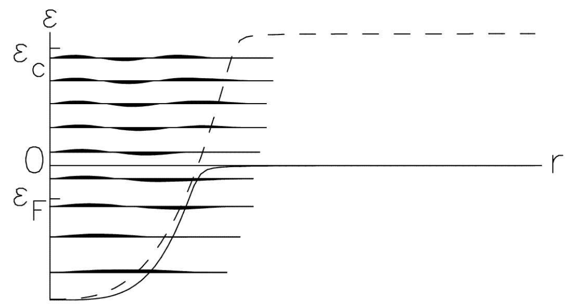
$b_i^\dagger$: quasi-particle states, including information on excitations.

HFB in canonical-basis method

HFB solutions can be expressed in the BCS form

$$|\Psi\rangle = \prod_{i=1}^{i_{\max}} \left(u_i + v_i\ a_i^\dagger\ a_{\bar{i}}^\dagger\right)|0\rangle$$
$$a_i^\dagger = \sum_s \int d^3r\ \psi_i(\vec{r},s)\ a^\dagger(\vec{r},s) \quad : \text{HFB canonical basis}$$

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



Exact when $i_{\max} = \frac{1}{2}\#\text{basis}$ (Bloch Messiah theorem)
One may neglect $v^2 \ll 1$ states to describe the ground state.
i.e., $i_{\max} = \mathcal{O}(A) \ll \#\text{basis}$ to a good approximation

h : Hartree-Fock Hamiltonian
$\tilde{h}$: Pairing Hamiltonian

Nature of the positive energy canonical basis

Positive-energy canonical basis

- are spatially localized by $\tilde{h}$.
- have a discrete spectrum.
- are determined by $\tilde{h}$, not by h.

Comparison of the two methods

method	#basis	orthogonality condition	pairig force
quasi particle	$\propto$ box vol.	redundant	δ-func, + dens. dep.
canonical basis	$\propto$ nucl. vol.	essential	+ mom. dep.

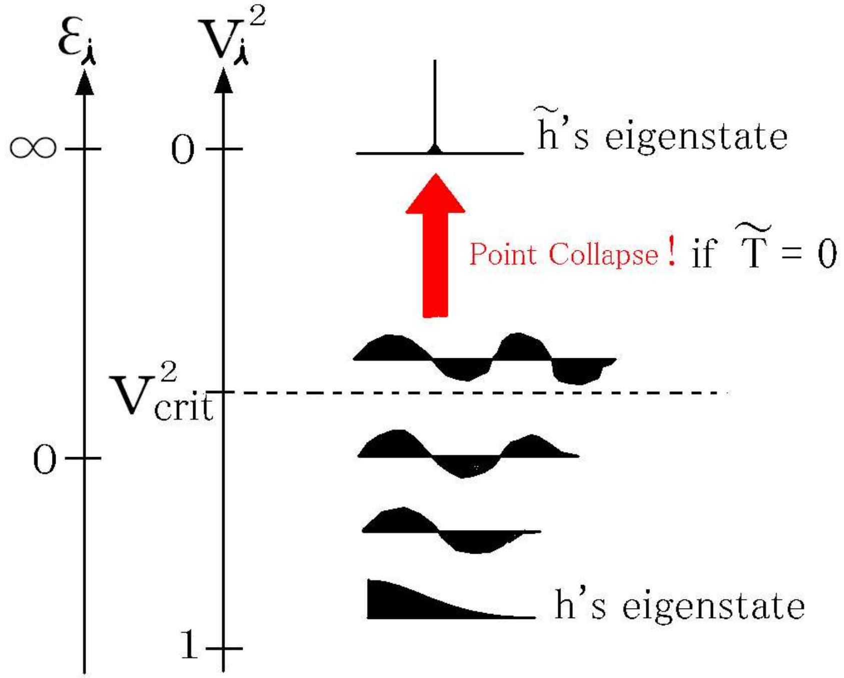
- Hamiltonian becomes state-dependent.

  $\Rightarrow$ Orthogonality among the canonical basis states should be explicitly taken care of.

- Necessity of momentum-dependent or finite-range pairing interaction

  $\Leftarrow$ Point collapse problem (see the next slide)

Point Collapse



<u>How to avoid the collapse</u>

- Sharp cutoff → too few orbitals
- Smooth cutoff → no q.p. Hamiltonian
- Density dependence
  → cannot prevent the collapse
- Pairing density dependence → OK
- Momentum dependence → OK

HFB with the Skyrme force

Mean-field interaction

$$\hat{v} = t_0(1+x_0P_\sigma)\delta + \frac{1}{2}t_1(1+x_1P_\sigma)(\vec{k}^2\delta + \delta\vec{k}^2) + t_2(1+x_2P_\sigma)\vec{k}\cdot\delta\vec{k}$$
$$+\frac{1}{6}\rho^\alpha t_3(1+x_3P_\sigma)\delta + iW(\vec{\sigma_1}+\vec{\sigma_2})\cdot\vec{k}\times\delta\vec{k}$$

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

$$\hat{v}_\mathrm{p} = v_\mathrm{p}\frac{1-P_\sigma}{2}\left\{\left[1-\frac{\rho}{\rho_\mathrm{c}}-\frac{\rho_\mathrm{n}-\rho_\mathrm{p}}{\rho'_\mathrm{c}}T_z-\left(\frac{\tilde{\rho}}{\tilde{\rho}_\mathrm{c}}\right)^2\right]\delta-\frac{1}{2{k_\mathrm{c}}^2}\left(\vec{k}^2\delta+\delta\vec{k}^2\right)\right\}$$

- v_p : overall strength, to be adjusted depending on the cutoff.
  Cutoff can be controlled by the number of (explicitly considered) canonical basis with $v^2 > 0$.

- $\rho_\mathrm{c} = 0.32\ \mathrm{fm}^{-1}$, $\rho'_\mathrm{c} = \tilde{\rho}_\mathrm{c} = \infty$: density dependence, insufficient information

- $k_\mathrm{c} = 2\ \mathrm{fm}^{-1}$: momentum dependence (=finite range effect), prevents the point collapse

Hamiltonian density for even-even nuclei

$$
\begin{aligned}
E = \int \mathcal{H} d\vec{r}, \quad \mathcal{H} &= \frac{\hbar^2}{2m}\left(\tau_{\rm n}+\tau_{\rm p}\right) \\
&+ C_1\left(\rho_{\rm n}^2+\rho_{\rm p}^2\right) + C_1'\rho_{\rm n}\rho_{\rm p} \\
&+ C_2\left(\rho_{\rm n}\tau_{\rm n}+\rho_{\rm p}\tau_{\rm p}\right) + C_2'\left(\rho_{\rm n}\tau_{\rm p}+\rho_{\rm p}\tau_{\rm n}\right) \\
&+ C_3\left(\rho_{\rm n}\vec{\nabla}^2\rho_{\rm n}+\rho_{\rm p}\vec{\nabla}^2\rho_{\rm p}\right) + C_3'\left(\rho_{\rm n}\vec{\nabla}^2\rho_{\rm p}+\rho_{\rm p}\vec{\nabla}^2\rho_{\rm n}\right) \\
&+ C_4\rho^\alpha\left(\rho_{\rm n}^2+\rho_{\rm p}^2\right) + C_4'\rho^\alpha\rho_{\rm n}\rho_{\rm p} \\
&+ C_5\left(\rho_{\rm n}\vec{\nabla}\cdot\vec{J}_{\rm n}+\rho_{\rm p}\vec{\nabla}\cdot\vec{J}_{\rm p}\right) + C_5'\left(\rho_{\rm n}\vec{\nabla}\cdot\vec{J}_{\rm p}+\rho_{\rm p}\vec{\nabla}\cdot\vec{J}_{\rm n}\right) \\
&+ C_6\tilde{\rho}_{\rm n}^2 + C_7\rho_{\rm n}\tilde{\rho}_{\rm n}^2 + C_7'\rho_{\rm p}\tilde{\rho}_{\rm n}^2 + C_8\tilde{\rho}_{\rm n}^4 + C_9\tilde{\rho}_{\rm n}\left(\tilde{\tau}_{\rm n}-\vec{\nabla}^2\tilde{\rho}_{\rm n}\right) \\
&+ C_6\tilde{\rho}_{\rm p}^2 + C_7\rho_{\rm p}\tilde{\rho}_{\rm p}^2 + C_7'\rho_{\rm n}\tilde{\rho}_{\rm p}^2 + C_8\tilde{\rho}_{\rm p}^4 + C_9\tilde{\rho}_{\rm p}\left(\tilde{\tau}_{\rm p}-\vec{\nabla}^2\tilde{\rho}_{\rm p}\right) \\
&+ C_{10}V_{\rm C}\rho_{\rm p} + C_{11}\rho_{\rm p}^{4/3}
\end{aligned}
$$

where

$$
\begin{aligned}
C_1 &= \tfrac{1}{4}t_0(1-x_0) & C_1' &= \tfrac{1}{2}t_0(2+x_0) \\
C_2 &= \tfrac{1}{8}\left(t_1(1-x_1)+3t_2(1+x_2)\right) & C_2' &= \tfrac{1}{8}\left(t_1(2+x_1)+t_2(2+x_2)\right) \\
C_3 &= \tfrac{3}{32}\left(t_1(x_1-1)+t_2(x_2+1)\right) & C_3' &= \tfrac{1}{32}\left(-3t_1(2+x_1)+t_2(2+x_2)\right) \\
C_4 &= \tfrac{1}{24}t_3(1-x_3) & C_4' &= \tfrac{1}{12}t_3(2+x_3) \\
C_5 &= -W & C_5' &= -\tfrac{1}{2}W \\
C_6 &= \tfrac{1}{4}v_{\rm P} & & \\
C_7 &= -\tfrac{1}{4}v_{\rm P}\left(\tfrac{1}{\rho_{\rm c}}+\tfrac{1}{\rho_{\rm c}'}\right) & C_7' &= -\tfrac{1}{4}v_{\rm P}\left(\tfrac{1}{\rho_{\rm c}}-\tfrac{1}{\rho_{\rm c}'}\right) \\
C_8 &= -\tfrac{1}{4}\tfrac{v_{\rm P}}{\tilde{\rho}_{\rm c}^2} & C_9 &= -\tfrac{1}{4}\tfrac{v_{\rm P}}{k_{\rm c}^2} \\
C_{10} &= \tfrac{1}{2} & C_{11} &= -\tfrac{3}{4}e^2\left(\tfrac{3}{\pi}\right)^{1/3}
\end{aligned}
$$

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

$$\tau_{\rm q}(\vec r) = 2\sum_{i>0,\sigma} v_{qi}^2 |\vec\nabla\psi_{qi}(\vec r,\sigma)|^2, \qquad \tilde\tau_{\rm q}(\vec r) = 2\sum_{i>0,\sigma} u_{qi}v_{qi}|\vec\nabla\psi_{qi}(\vec r,\sigma)|^2,$$

$$\rho_{\rm q}(\vec r) = 2\sum_{i>0,\sigma} v_{qi}^2|\psi_{qi}(\vec r,\sigma)|^2, \qquad \tilde\rho_{\rm q}(\vec r) = 2\sum_{i>0,\sigma} u_{qi}v_{qi}|\psi_{qi}(\vec r,\sigma)|^2$$

$$\vec\nabla\cdot\vec J_{\rm q} = \frac{2}{i}\sum_{i>0,\sigma,\sigma'} v_{qi}^2\vec\nabla\psi_{qi}^*(\vec r,\sigma)\times\vec\nabla\psi_{qi}(\vec r,\sigma')\cdot\langle\sigma|\vec\sigma|\sigma'\rangle$$

Effective masses and single-particle potentials

$$\begin{aligned}
B_{\rm n} &= \frac{\hbar^2}{2m} + C_2\rho_{\rm n} + C_2'\rho_{\rm p}\\
\tilde B_{\rm n} &= C_9\tilde\rho_{\rm n}\\
V_{\rm n} &= 2C_1\rho_{\rm n} + C_1'\rho_{\rm p} + C_2\tau_{\rm n} + C_2'\tau_{\rm p} + 2C_3\vec\nabla^2\rho_{\rm n} + 2C_3'\vec\nabla^2\rho_{\rm p}\\
&\quad +\rho^{\alpha-1}\left[(\alpha+2)C_4\rho_{\rm n}^2 + (\alpha C_4 + C_4')\rho_{\rm p}^2 + (2C_4 + (\alpha+1)C_4')\rho_{\rm n}\rho_{\rm p}\right]\\
&\quad +C_5\vec\nabla\cdot\vec J_{\rm n} + C_5'\vec\nabla\cdot\vec J_{\rm p} + C_7\tilde\rho_{\rm n}^2 + C_7'\tilde\rho_{\rm p}^2\\
\vec W_{\rm n} &= -C_5\vec\nabla\rho_{\rm n} - C_5'\vec\nabla\rho_{\rm p}\\
\tilde V_{\rm n} &= 2C_6\tilde\rho_{\rm n} + 2C_7\rho_{\rm n}\tilde\rho_{\rm n} + 2C_7'\rho_{\rm p}\tilde\rho_{\rm n} + 4C_8\tilde\rho_{\rm n}^3 + C_9\left(\tilde\tau_{\rm n} - 2\vec\nabla^2\tilde\rho_{\rm n}\right)
\end{aligned}$$

State dependent Hamiltonian

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

Approach to the drip line (and beyond)

isotope chain:

Si(Z=14), $6 \leq N \leq 32$ have bound states

Mean filed:

SIII force, ls and Coulomb excluded.

Pairing force:

$k_c = 2$ fm^{-1}, $\rho_c = 0.32$ fm^{-3}.

v_p(MeV fm^3)	-680	-780	-880
$\Delta_n(N = 28)$(MeV)	1.4	2.0	3.0

Mainly, $v_p = -780$ is used.

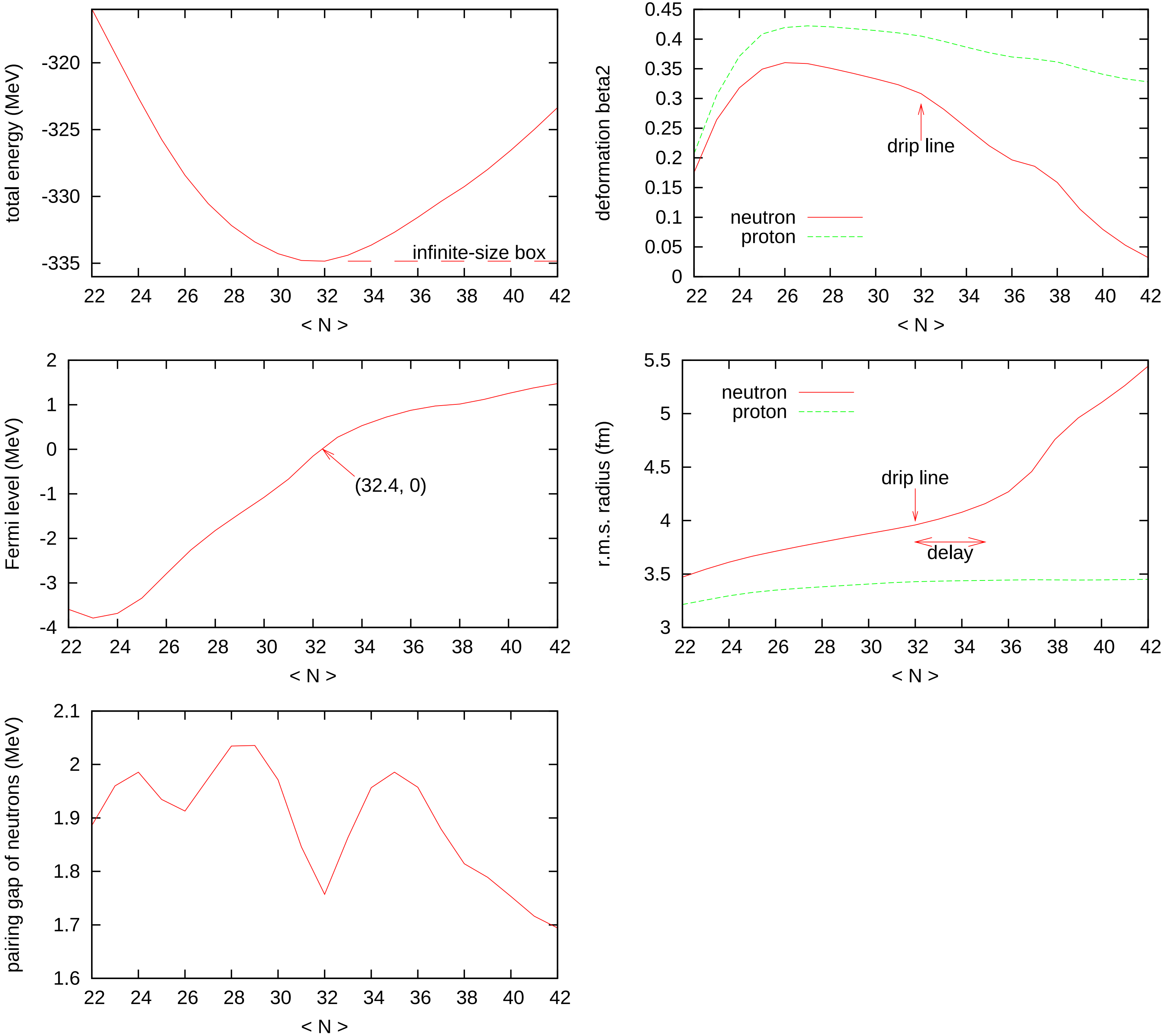
Box:

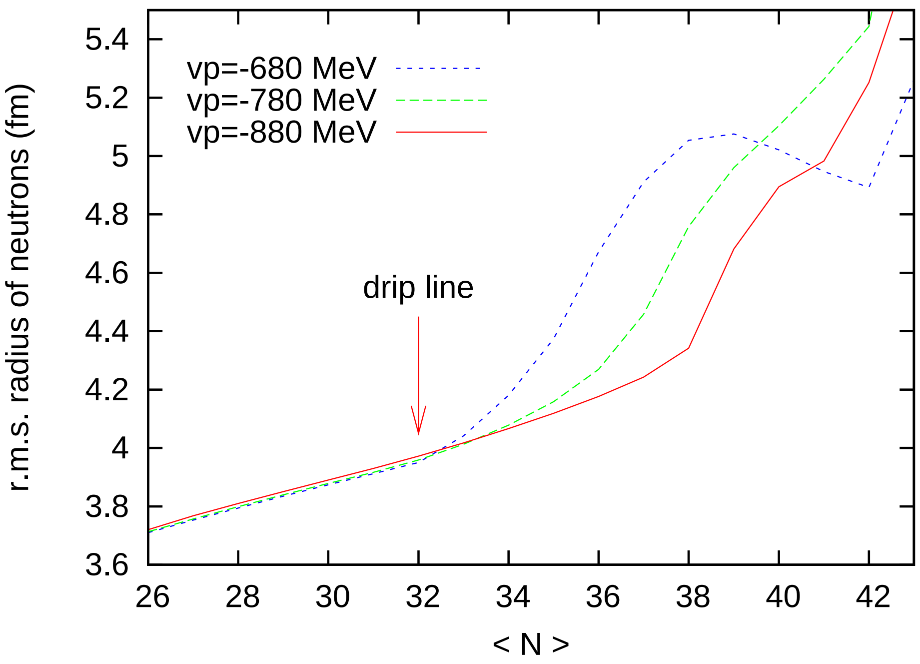
$L = 32$ fm, $\Delta x = 0.8$ fm

The number of canonical basis states:

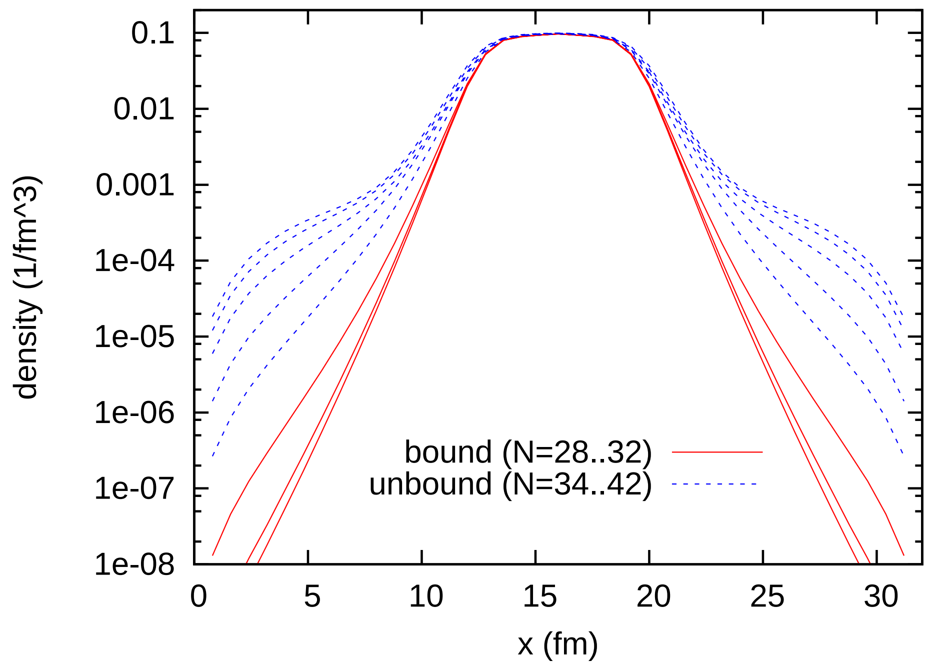
neutrons : 60×2 (2 for spin $\uparrow$ and $\downarrow$)

protons : $21 \times 2 \longrightarrow$ mostly in the normal state


total energy (MeV)
-320
-325
-330
-335
infinite-size box
22
24
26
28
30
32
34
36
38
40
42
< N >
deformation beta2
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
drip line
neutron
proton
< N >
Fermi level (MeV)
2
1
0
-1
-2
-3
-4
(32.4, 0)
< N >
r.m.s. radius (fm)
5.5
5
4.5
4
3.5
3
neutron
proton
drip line
delay
< N >
pairing gap of neutrons (MeV)
2.1
2
1.9
1.8
1.7
1.6
< N >

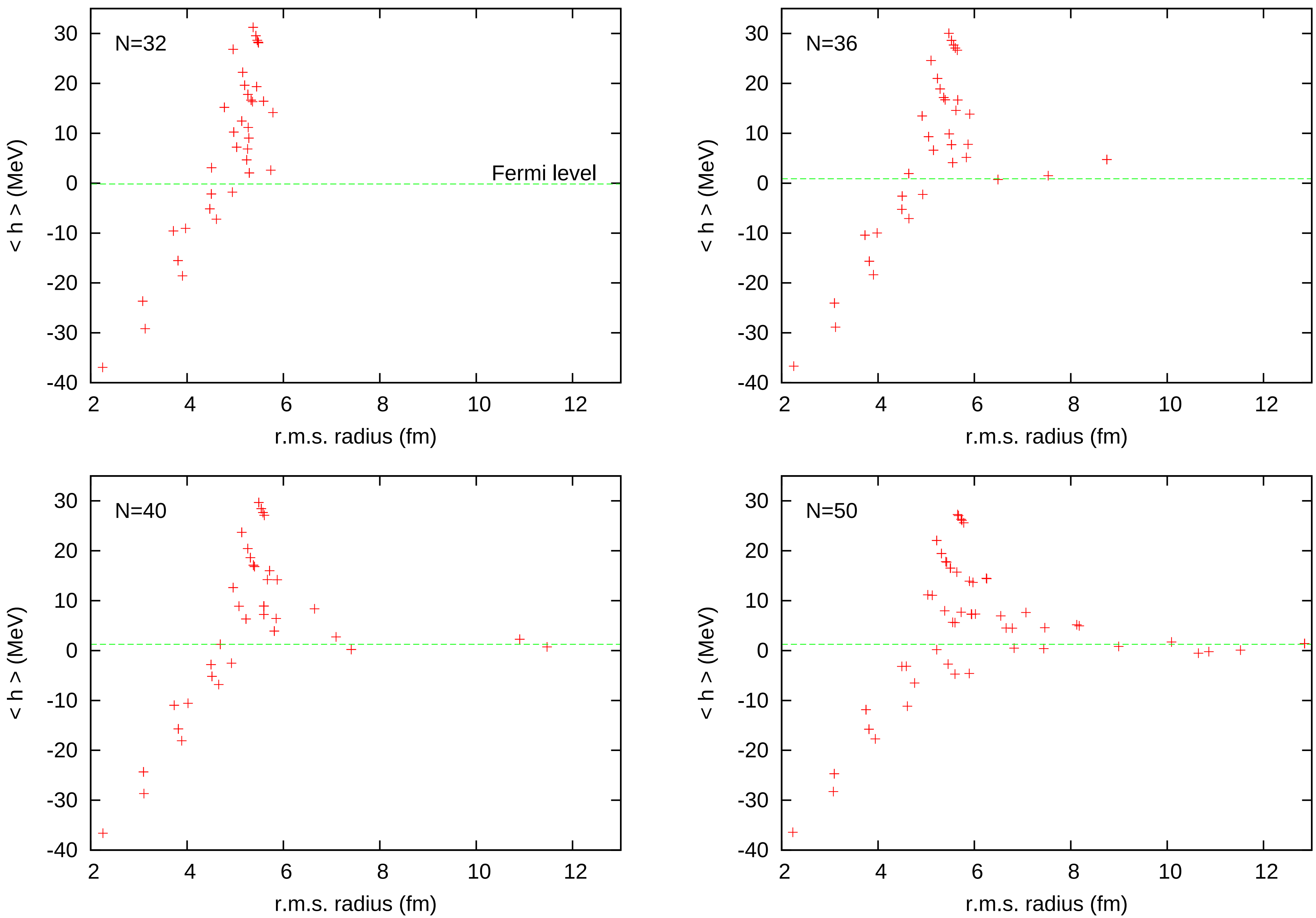


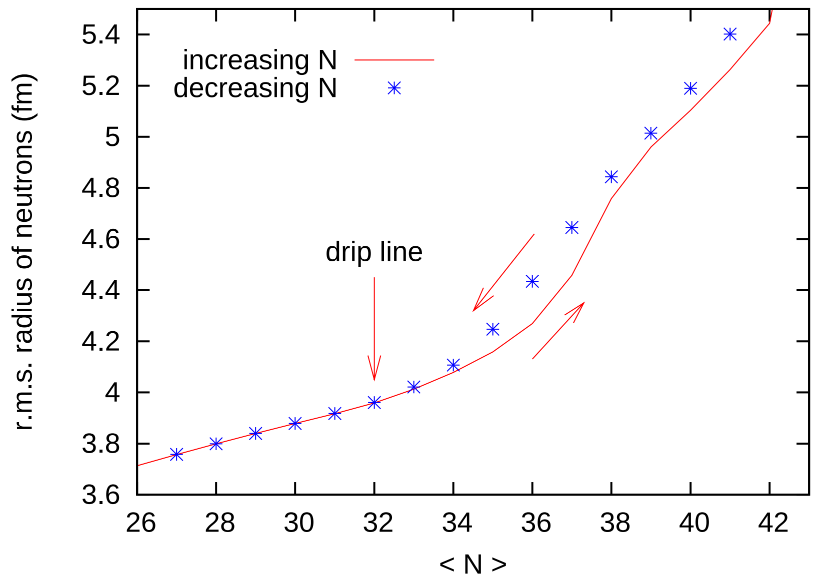
Stronger pairings lead to longer delays of dislocalization.



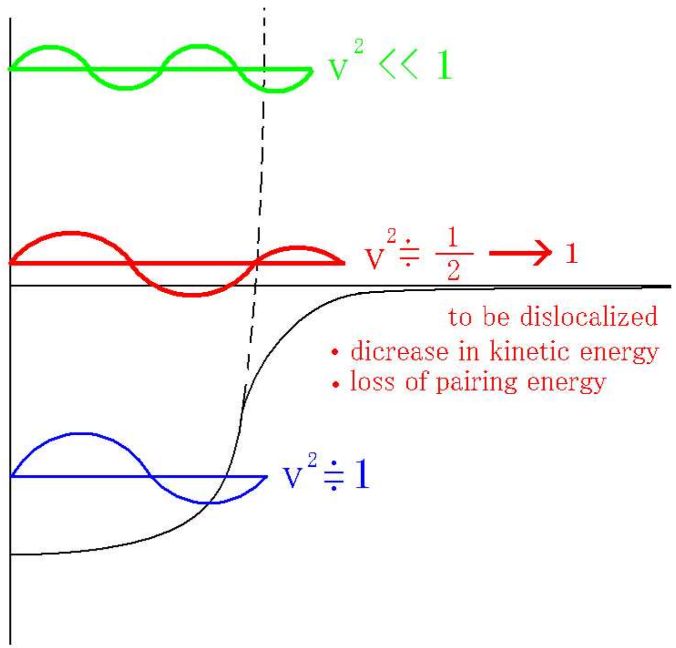
$v_p = -780$ MeV fm^3

Canonical basis states of neutrons

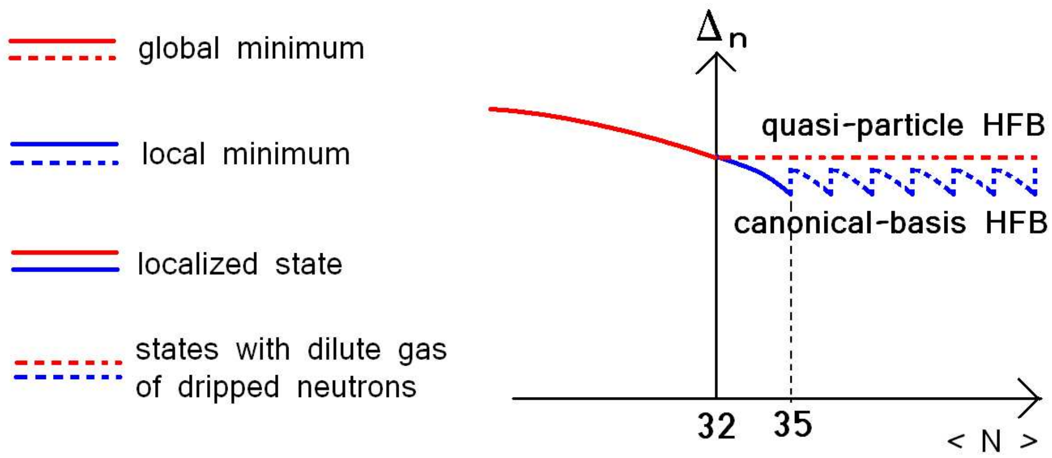




r.m.s. radius of neutrons (fm)
5.4
5.2
5
4.8
4.6
4.4
4.2
4
3.8
3.6
26
28
30
32
34
36
38
40
42
< N >
increasing N
decreasing N
drip line



$v^2 << 1$
$v^2 \doteqdot \frac{1}{2} \rightarrow 1$
$v^2 \doteqdot 1$
to be dislocalized
• dicrease in kinetic energy
• loss of pairing energy



global minimum
local minimum
localized state
states with dilute gas of dripped neutrons
Δ_n
quasi-particle HFB
canonical-basis HFB
32
35
< N >

Summary

1. Canonical-basis HFB method is presented.
   It is a much more economical way to express HFB ground states of neutron rich nuclei than expressing them as quasiparticle vacua.
   Positive energy canonical-basis states are obtained as the bound states of the pairing Hamiltonian.
   Consequently, they are guaranteed to be spatially localized and form a discrete spectrum.

2. The code has been extended to treat $N \neq Z$ systems.
   Spin-orbit and Coulomb forces are not considered.

3. No difficulties are encountered in reaching the neutron drip line.
   Approximate localized solutions for nearly bound systems can be obtained. It is probably not only for the finite-sized box but for the method to obtain solutions.

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