Donshu work shop at KEK, Tsukuba, 2005/3/21
JPS meeting at Tokyo University of Science, Noda, 24pWG-14, 2005/3/24

# Approximate spatially-localized HFB solutions for nuclei beyond the neutron drip line

## — Canonical-basis HFB method —

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Demands

1. Pairing in the continuum $\epsilon_{\rm F} > -\frac{1}{2}\hbar\omega_{\rm osc}$ $\frac{10^4}{2}$ nuclides
2. Long tail for large $r$ $\epsilon_{\rm F} > -1$ MeV halo
3. Deformation all but near spherical magics

Answer

**Coordinate-space Hartree-Fock-Bogoliubov**

such as 3D Cartesian mesh not HF+BCS

feasible for Skyrme force

but, How to solve ?

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

## Hartree-Fock

$$
\begin{aligned}
|\psi\rangle &= \prod_{i=1}^{A} a_i^\dagger |0\rangle \\
a_i^\dagger &= \sum_s \int d^3r\ \psi_i(\vec{r},s)\ a^\dagger(\vec{r},s) \quad : \text{single-particle state}
\end{aligned}
$$

Variation with $A$ wavefunctions $\{\psi_i\}_{i=1,\cdots,A}$
Orthonormality condition $\langle\psi_i|\psi_j\rangle = \delta_{ij}$

$$
\frac{\delta E}{\delta\psi_i^*} = h\psi_i = \epsilon_i\psi_i
$$

## HFB in quasi-particle method

$$
\begin{aligned}
|\psi\rangle &= \prod_{i=1}^{\#\text{basis}} b_i|0\rangle \\
b_i &= \sum_s \int d^3r \left\{\phi_i^*(\vec{r},s)\ a(\vec{r},s) + \psi_i(\vec{r},s)\ a^\dagger(\vec{r},s)\right\} \ : \text{quasi-particle state}
\end{aligned}
$$

Variation with $2\times\#$basis wavefunctions $\{\phi_i,\psi_i\}_{i=1,\cdots,\#\text{basis}}$
Constraints: $\langle\phi_i|\phi_j\rangle + \langle\psi_i|\psi_j\rangle = \delta_{ij}$ and $\sum\langle\psi_i|\psi_i\rangle = A$

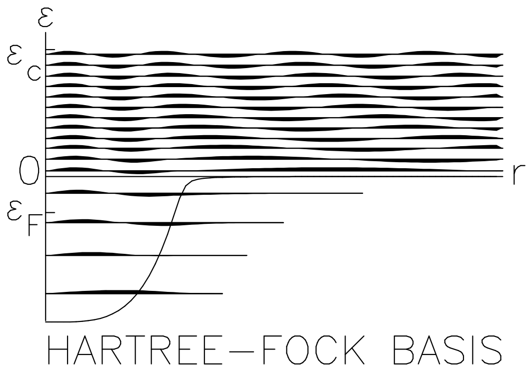
$$
\begin{pmatrix} -h & \tilde{h} \\ \tilde{h} & h \end{pmatrix} \begin{pmatrix} \phi_i \\ \psi_i \end{pmatrix} = \epsilon_i \begin{pmatrix} \phi_i \\ \psi_i \end{pmatrix}
$$

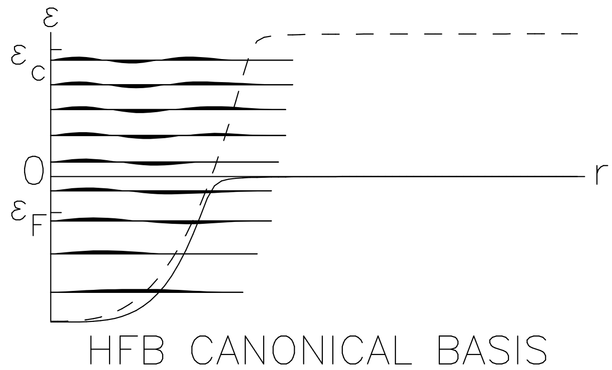
## HFB in canonical-basis method

HFB solutions can be expressed in the BCS form (Bloch Messiah Theorem):

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

Variation with $\{\psi_i,(\bar{\psi}_i),u_i\}_{i=1,\cdots,i_{\max}}$
Constraints: $\langle\psi_i|\psi_j\rangle = \delta_{ij}$、 $u_i^2+v_i^2=1$ and $2\sum v_i^2 = A$
Exact when $i_{\max} = \frac{1}{2}\#$basis (Bloch Messiah theorem)
$i \le i_{\max} = \mathcal{O}(A) \ll \#$basis : a good approximation




(≈ quasi-particle states)
includes information on excitations.

One may neglect $v^2 \ll 1$ states
to describe the ground state.

$$\frac{\delta E}{\delta \psi_i^*} = \mathcal{H}_i \psi_i = \sum_j \lambda_{ij} \psi_j$$

Hamiltonian becomes state-dependent :

$$\mathcal{H}_i = v_i^2 h + u_i v_i \tilde{h}$$

$h$ : Hartree-Fock Hamiltonian

$\tilde{h}$ : Pairing Hamiltonian

It is $\tilde{h}$ which governs positive-energy canonical basis.

⇑ not $h$

⇑ Resonances of $h$ cannot replace them.

## How to obtain HFB solutions in the canonical-basis form

$$|\Psi\rangle = \prod_{i=1}^{K} \left( u_i + v_i \, a_i^\dagger \, a_{\bar{i}}^\dagger \right) |0\rangle \tag{1}$$

Minimize $E = \langle \Psi | H | \Psi \rangle$ by varying $v_i$ and $\psi_i(\vec{r})$ under constraints,

$$4 \sum_{i=1}^{K} v_i^2 = A \tag{2}$$

$$\langle \psi_i | \psi_j \rangle = \delta_{ij} \quad (1 \le i \le j \le K) \tag{3}$$

Equivalently, minimize Routhian $R$ without constraints,

$$R = E - \epsilon_{\rm Fermi} \cdot 4 \sum_{i=1}^{K} v_i^2 - \sum_{i=1}^{K} \sum_{j=1}^{K} \lambda_{ij} \left\{ \langle \psi_i | \psi_j \rangle - \delta_{ij} \right\}. \tag{4}$$

- $\lambda_{ij} = \lambda_{ji}^*$ : $\frac{1}{2}K(K+1)$ constraints $\Longleftrightarrow$ $K^2$ multipliers
- $\lambda_{ij}$ : not constants but functionals

$$\frac{\partial R}{\partial v_i} = 0 \;\Rightarrow\; v_i^2 = \frac{1}{2} - \frac{1}{2} \frac{h_{ii} - \epsilon_{\rm Fermi}}{\sqrt{(h_{ii} - \epsilon_{\rm Fermi})^2 + \tilde{h}_{ii}^2}}, \tag{5}$$

$$\frac{\delta R}{\delta \psi_i^*} = \mathcal{H}_i \psi_i - \sum_{j=1}^{K} \lambda_{ij} \psi_j - \sum_{j=1}^{K} \sum_{k=1}^{K} \frac{\delta \lambda_{jk}}{\delta \psi_i^*} \left\{ \langle \psi_j | \psi_k \rangle - \delta_{jk} \right\} = 0, \tag{6}$$

- $\mathcal{H}_i = v_i^2 h + u_i v_i \tilde{h}$ is state-dependent.

$\Rightarrow$ Orthogonality conditions are essential.

$\Leftrightarrow$ HF solution is a saddle without $\lambda_{ij}$: $h|i\rangle = \epsilon_i |i\rangle \Rightarrow \langle i | j \rangle = \delta_{ij}$

Eq. (6) at the solution (where $\langle \psi_i | \psi_j \rangle = \delta_{ij}$), $\Rightarrow$

$$\lambda_{ij} = \langle \psi_j | \mathcal{H}_i | \psi_i \rangle \quad \text{at the solution.} \tag{7}$$

$\lambda_{ij} = \lambda_{ji}^* \Rightarrow \langle \psi_j | \mathcal{H}_i | \psi_i \rangle = \langle \psi_i | \mathcal{H}_j | \psi_j \rangle^* = \langle \psi_j | \mathcal{H}_j | \psi_i \rangle$ at the solution.

$$\lambda_{ij} = \frac{1}{2} \langle \psi_j | \left( \mathcal{H}_i + \mathcal{H}_j \right) | \psi_i \rangle \quad : \text{hermite everywhere} \tag{8}$$

- Acceleration of the convergence

  Imaginary-time evolution method to first order in $\Delta\tau$:

$$\psi_i \longrightarrow \psi_i - \Delta\tau \frac{\delta R}{\delta \psi_i^*} \tag{9}$$

More general gradient method using $\chi_i \equiv \alpha_i^{-1/2} \psi_i$:

$$\chi_i \longrightarrow \chi_i - \Delta\tau \frac{\delta R}{\delta \chi_i^*} \tag{10}$$

which is equivalent to

$$\psi_i \to \psi_i - \alpha_i \Delta\tau \frac{\delta R}{\delta \psi_i^*} \tag{11}$$

We take $\alpha_i = \min(\frac{1}{v_i^2},\ \frac{5}{u_i v_i})$ so that

$$\alpha_i h_i = \begin{cases} h & : \text{for deep hole states} \\ 5\tilde{h} & : \text{for high-energy particle states} \end{cases}$$

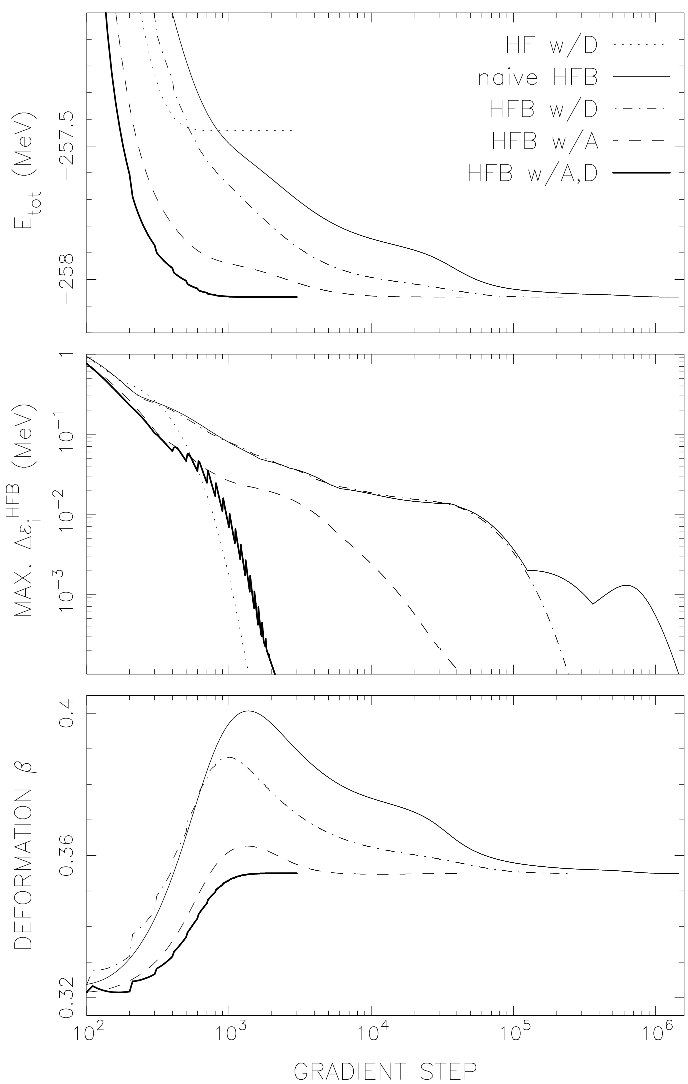
- Improved $\lambda_{ij}$

  $\delta\lambda_{ij}/\delta\psi_k$ is neglected

  $\Rightarrow$ Orthogonality should be conserved during the gradient-method iterations.

$$\lambda_{ij} = \frac{1}{\alpha_i + \alpha_j} \langle\psi_j| \left(\alpha_i \mathcal{H}_i + \alpha_j \mathcal{H}_j\right) |\psi_i\rangle$$

$$\Rightarrow \langle\psi_i|\psi_j\rangle - \delta_{ij} = \mathcal{O}\left((\Delta\tau)^2\right)$$



## HFB with the Skyrme force

**Skyrme force**

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

SIII parameters and $W=0$ for the mean-field (HF) potential.
S=0 T=1 terms for the pairing force:

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

**Hamiltonian density for even-even $N{=}Z$ nuclei:**

$$
\begin{aligned}
E &= \int \mathcal{H} d\vec{r} \\
\mathcal{H} &= \frac{\hbar^2}{2m}\tau + \frac{3}{8}t_0\rho^2 + \tfrac{3t_1+5t_2+4t_2x_2}{16}\rho\tau + \tfrac{-9t_1+5t_2+4t_2x_2}{64}\rho\triangle\rho + \frac{1}{16}t_3\rho^{2+\alpha} \\
&\quad + \frac{1}{8}v_{\mathrm{p}}\left\{\left(1-\frac{\rho}{\rho_{\mathrm{c}}}-\left(\frac{\tilde{\rho}}{\tilde{\rho}_{\mathrm{c}}}\right)^2\right)\tilde{\rho}^2 - \frac{1}{k_{\mathrm{c}}^2}\left(\tilde{\tau}-\triangle\tilde{\rho}\right)\tilde{\rho}\right\}
\end{aligned}
$$

where

$$
\begin{aligned}
\tau(\vec{r}) &= 4\sum_{i=1}^{K} v_i^2|\vec{\nabla}\psi_i(\vec{r})|^2, \qquad & \tilde{\tau}(\vec{r}) &= 4\sum_{i=1}^{K} u_iv_i|\vec{\nabla}\psi_i(\vec{r})|^2, \\
\rho(\vec{r}) &= 4\sum_{i=1}^{K} v_i^2|\psi_i(\vec{r})|^2, \qquad & \tilde{\rho}(\vec{r}) &= 4\sum_{i=1}^{K} u_iv_i|\psi_i(\vec{r})|^2
\end{aligned}
$$

Effective masses and single-particle potentials:

$$
\begin{aligned}
B &= \frac{\hbar^2}{2m} + \tfrac{3t_1+5t_2+4t_2x_2}{16}\rho, \qquad & V &= \tfrac{3}{4}t_0\rho + \tfrac{2+\alpha}{16}t_3\rho^{1+\alpha} + (\cdots)\tau + (\cdots)\triangle\rho - \frac{v_{\mathrm{p}}}{8\rho_{\mathrm{c}}}\tilde{\rho}^2 \\
\tilde{B} &= -\frac{v_{\mathrm{p}}}{8k_{\mathrm{c}}^2}\tilde{\rho}, \qquad & \tilde{V} &= \frac{1}{4}v_{\mathrm{p}}\left\{\left(1-\frac{\rho}{\rho_{\mathrm{c}}}-2\left(\frac{\tilde{\rho}}{\tilde{\rho}_{\mathrm{c}}}\right)^2\right)\tilde{\rho} - \frac{1}{2k_{\mathrm{c}}^2}\tilde{\tau} + \frac{1}{k_{\mathrm{c}}^2}\triangle\tilde{\rho}\right\}
\end{aligned}
$$

State dependent Hamiltonian:

$$
\begin{aligned}
h &= -\vec{\nabla}\cdot B\vec{\nabla} + V && : \text{ mean-field Hamiltonian} \\
\tilde{h} &= -\vec{\nabla}\cdot \tilde{B}\vec{\nabla} + \tilde{V} && : \text{ pairing Hamiltonian} \\
\mathcal{H}_i &= v_i^2 h + u_iv_i\tilde{h} && : \text{ Hamiltonian of } i\text{th canonical orbital}
\end{aligned}
$$

# $t_1$ term in the pairing interaction

Finite-range effects in s-wave relative motion

⇓

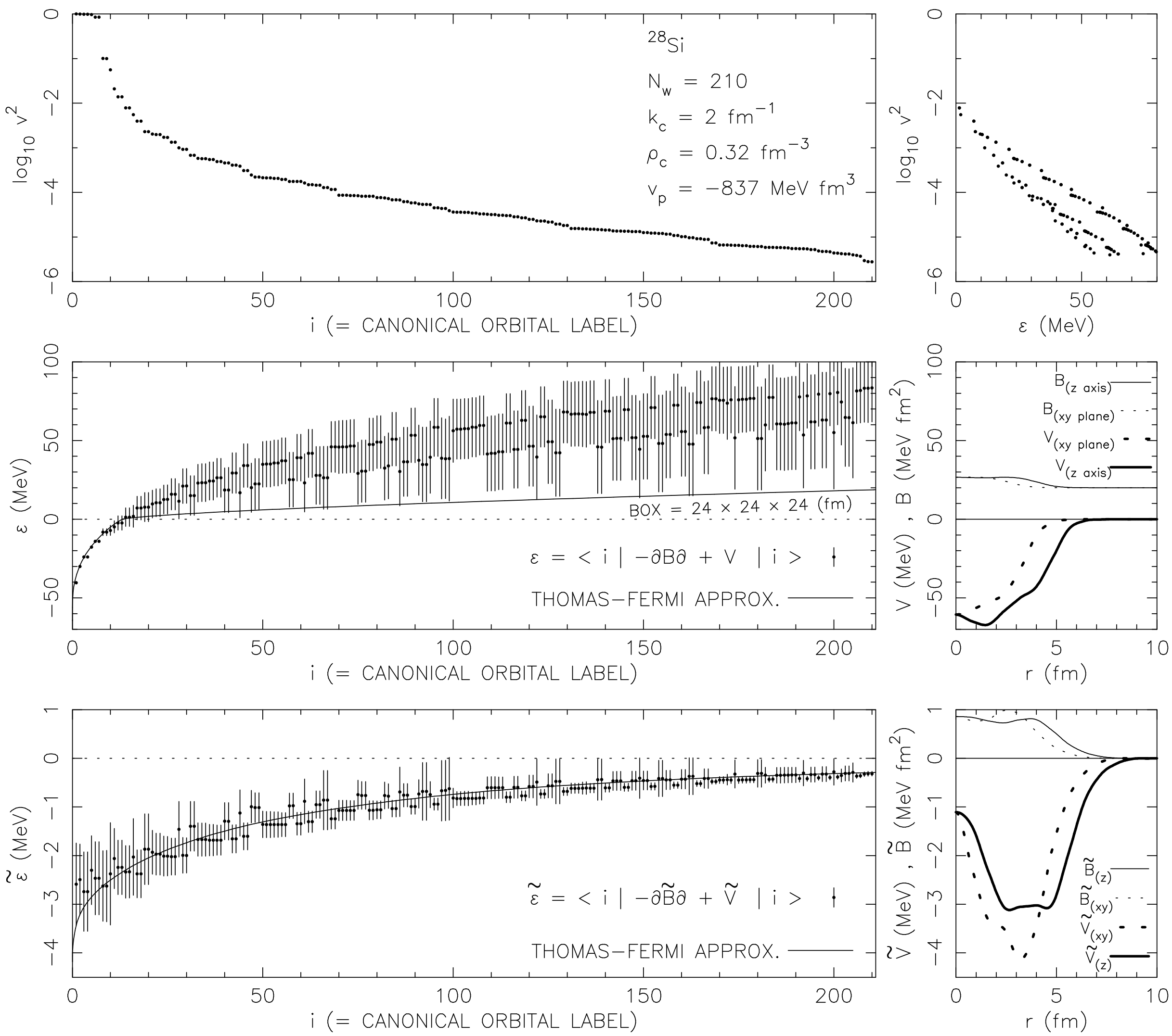
## $t_1$ term

⇓

Kinetic energy term in $\tilde{h}$

**1.** prevents point collapse of a high-lying canonical orbital

**2.** allows a simple understanding of the nature of the canonical orbitals



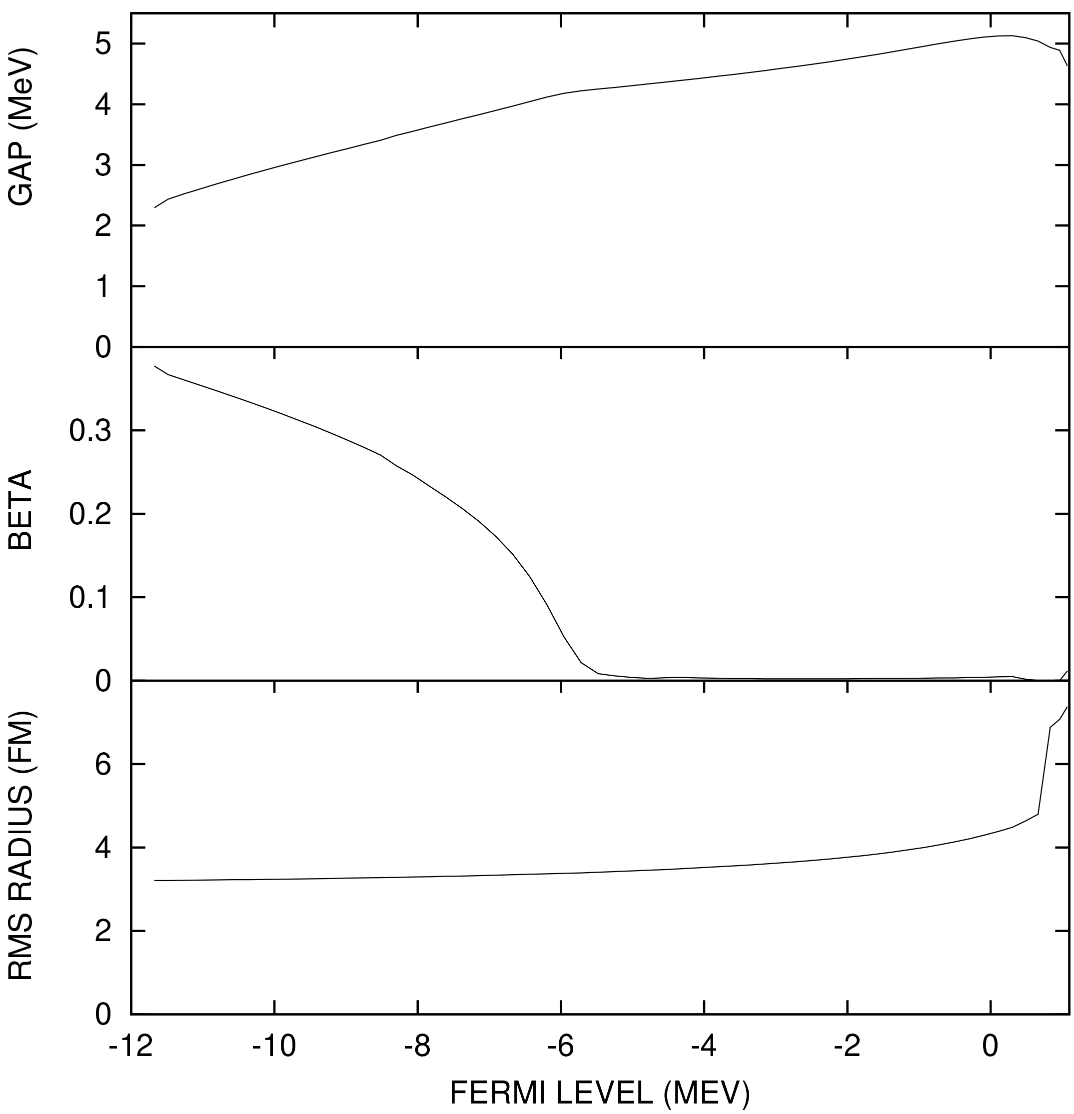
## Simulation of the approach to the drip line (and beyond).

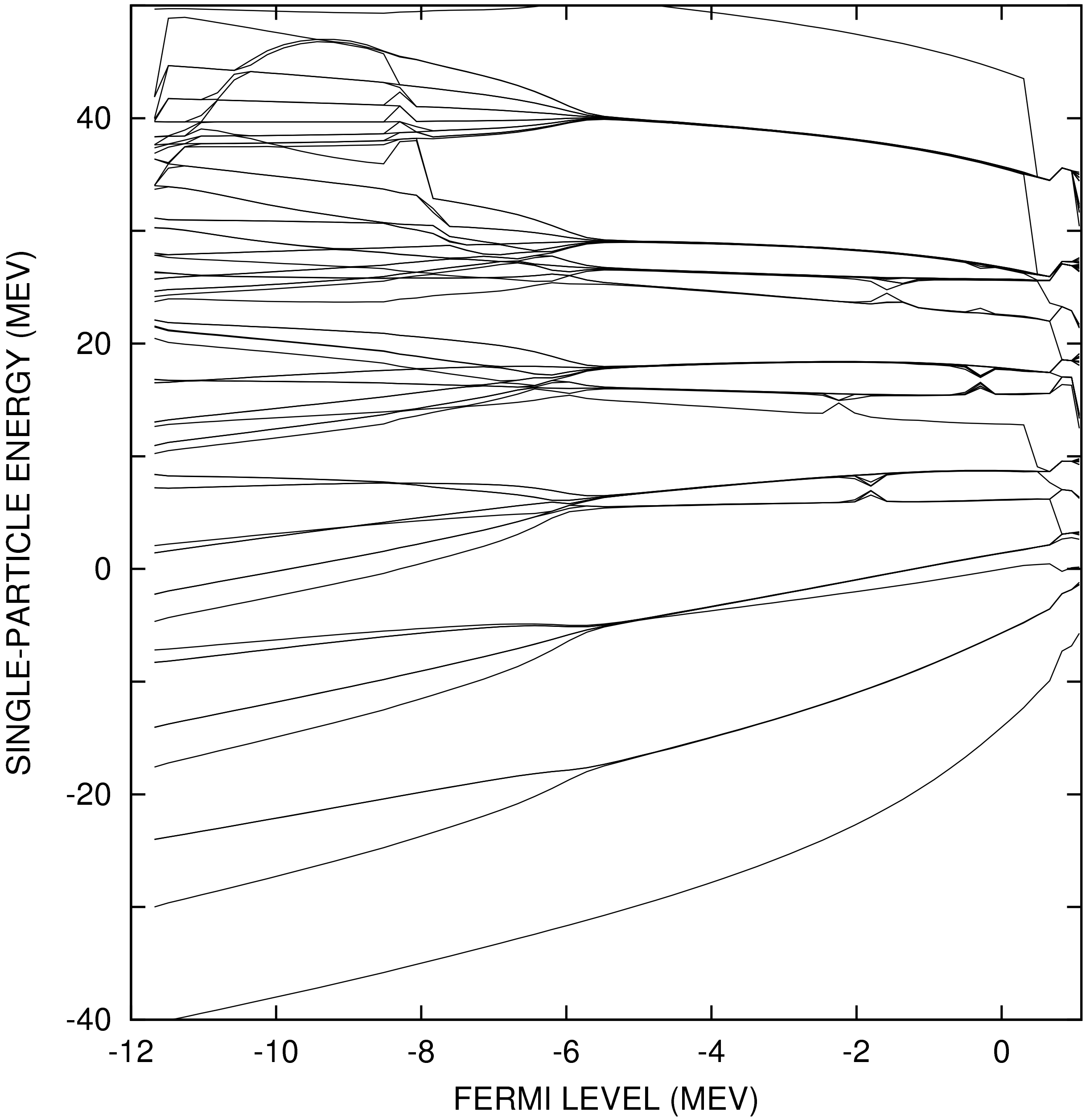
$N$=$Z$=14, modified SIII force ($t_0\uparrow, t_3\downarrow$), ls and Coulomb excluded.
Pairing force: $v_{\rm p} = -880$ MeV fm$^3$, $k_{\rm c} = 2$ fm$^{-1}$, $\rho_{\rm c} = 0.32$ fm$^{-3}$.
box: $L = 40$ fm, $\Delta x = 0.8$ fm, #w.f.=70 × 4

$$e = \frac{\mathcal{H}}{\rho} = \frac{\hbar^2}{2m}\beta\rho^{2/3} + \frac{3}{8}t_0\rho + \frac{1}{16}t_3\rho^2, \qquad \beta = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}$$

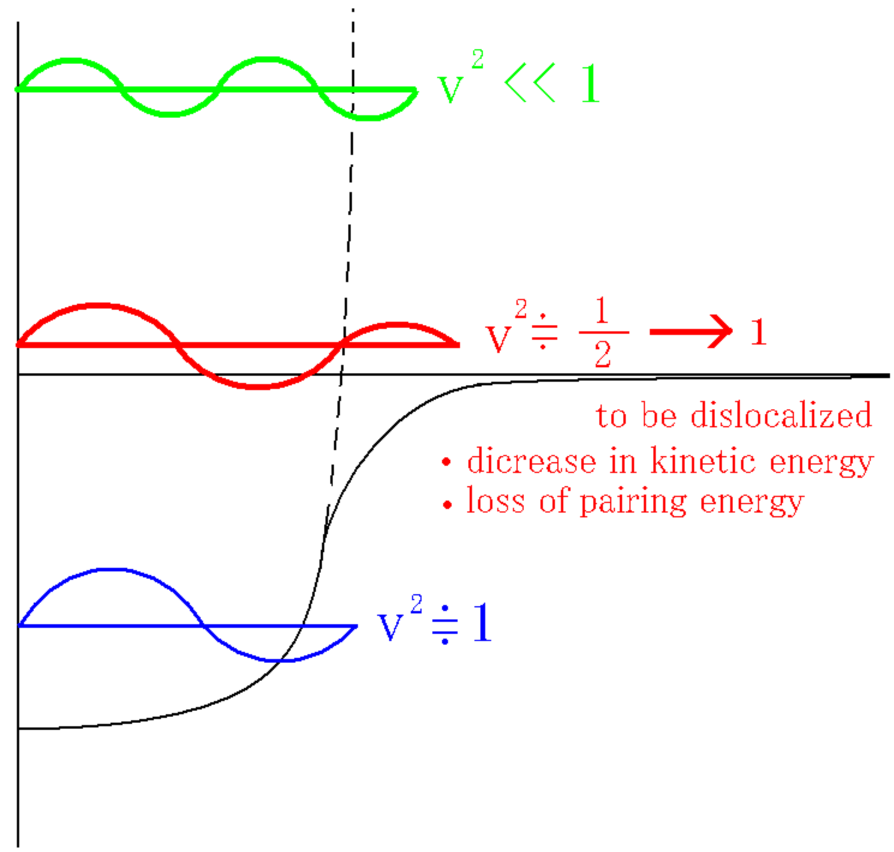
$\frac{de}{d\rho} = 0$ at $\rho = \rho_{\rm eq}$, $\qquad \lambda = \frac{d\mathcal{H}}{d\rho} = \frac{\mathcal{H}}{\rho}$ at $\rho = \rho_{\rm eq}$

$$t_3 = -\frac{3}{\rho_{\rm eq}}t_0 - \frac{\hbar^2}{2m}\frac{16\beta}{3}\rho_{\rm eq}^{-4/3}, \qquad \rho_{\rm eq} = 0.145{\rm fm}^{-3}$$

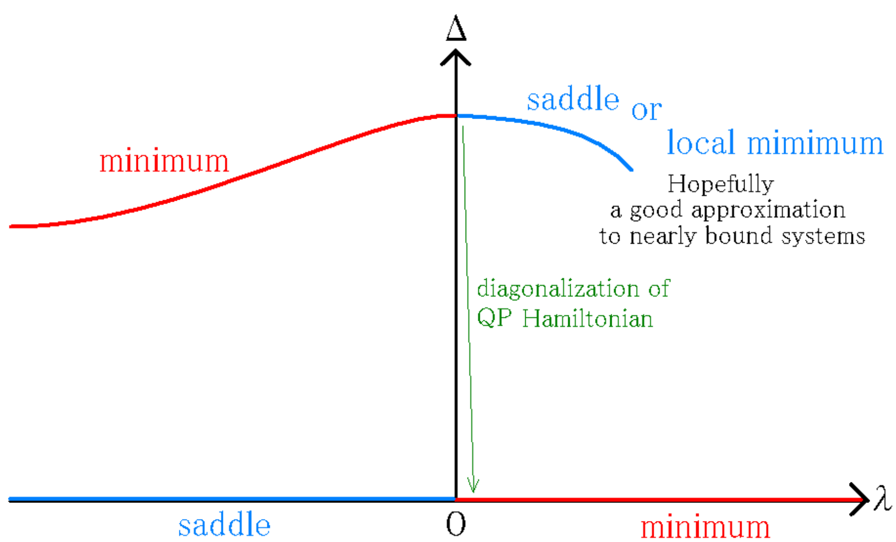





- No drastic changes are observed in crossing the drip line.
- For $\lambda < 0$, it is related to the Pairing Anti Halo effect
- For $\lambda > 0$ , the true ground state must be a dislocalized state according to quasi-particle HFB.
- Canonical-basis HFB can also give a spatially localized local-minimum solution, which may be, hopefully, a good approximation to nealy bound systems.



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

Δ
saddle or
local mimimum
minimum
Hopefully
a good approximation
to nearly bound systems
diagonalization of
QP Hamiltonian
saddle
0
minimum
λ

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