Hartree-Fock-Bogoliubov (HFB) Theory

HF+BCS method: first solve HF, and then introduce the Bogoliubov transformation

$$H = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + V_{\mathrm{HF}}(i)\right) + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i,\boldsymbol{r}_j) - \sum_i V_{\mathrm{HF}}(i)$$

$$= \sum_k \epsilon_k a_k^\dagger a_k + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i,\boldsymbol{r}_j) - \sum_i V_{\mathrm{HF}}(i)$$

→ $\alpha_\nu^\dagger = u_\nu a_\nu^\dagger - v_\nu a_{\bar{\nu}}$ (defined with HF basis)

→ $\alpha_\nu|BCS\rangle = 0$

Hartree-Fock-Bogoliubov (HFB) method: generalizes and unifies HF and BCS methods

generalized Bogoliubov transformation

$$\beta_k^\dagger = \sum_{k'} U_{k'k}\, c_{k'}^\dagger + V_{k'k}\, c_{k'}$$

→ $\beta_k|HFB\rangle = 0$

Hartree-Fock-Bogoliubov (HFB) method: generalizes and unifies HF and BCS methods

generalized Bogoliubov transformation

$$\beta_k^\dagger = \sum_{k'} U_{k'k}\, c_{k'}^\dagger + V_{k'k}\, c_{k'}$$

$$\{\beta_k, \beta_{k'}^\dagger\} = \delta_{k,k'} \Rightarrow U^\dagger U + V^\dagger V = 1$$

$$\beta_k \,|HFB\rangle = 0$$

$$|HFB\rangle = \prod_k \beta_k |0\rangle$$

(note) in the normal fluid phase:

$$|HF\rangle = \prod_k a_k^\dagger |0\rangle, \qquad a_k = \sum_{k'} V_{k'k} c_{k'}$$

Hamiltonian in the second quantization representation:

$$H = \sum_{1,2} t_{12}\, c_1^\dagger\, c_2 + \frac{1}{4} \sum_{1,2,3,4} \bar{v}_{1234}\, c_1^\dagger\, c_2^\dagger\, c_4\, c_3$$

$$\bar{v}_{1234} = \langle 12|v|34\rangle - \langle 12|v|43\rangle$$

$$|HFB\rangle = \prod_k \beta_k |0\rangle \qquad \beta_k^\dagger = \sum_{k'} U_{k'k}\, c_{k'}^\dagger + V_{k'k}\, c_{k'}$$

$$\langle HFB|H - \lambda\hat{N}|HFB\rangle = Tr((t-\lambda)\rho + \Gamma\rho/2 - \Delta\kappa^*/4)$$

$$\rho_{kk'} = \langle HFB|c_{k'}^\dagger c_k|HFB\rangle = (V^*V^T)_{kk'}$$

$$\kappa_{kk'} = \langle HFB|c_{k'} c_k|HFB\rangle = (V^*U^T)_{kk'}$$

$$\langle HFB|H-\lambda\hat{N}|HFB\rangle = Tr((t-\lambda)\rho+\Gamma\rho/2-\Delta\kappa^*/4)$$

density

$$\rho_{kk'} = \langle HFB|c^\dagger_{k'}c_k|HFB\rangle = (V^*V^T)_{kk'}$$

abnormal density

$$\kappa_{kk'} = \langle HFB|c_{k'}c_k|HFB\rangle = (V^*U^T)_{kk'} = -(UV^\dagger)_{kk'}$$

mean-field potential

$$\Gamma_{kk'} = \sum_{qq'} \bar{v}_{kq'k'q}\,\rho_{qq'}$$

pairing potential

$$\Delta_{kk'} = \frac{1}{2}\sum_{qq'} \bar{v}_{kk'qq'}\,\kappa_{qq'}$$

HFB Equations

$$\left\{ \begin{array}{lcl} \dfrac{\delta}{\delta V^*_{k'k}} \left[\langle H - \lambda \widehat{N} \rangle + E_k \left(\sum_{k'} U^\dagger_{kk'} U_{k'k} + V^\dagger_{kk'} V_{k'k} \right) \right] & = & 0 \\ \dfrac{\delta}{\delta U^*_{k'k}} \left[\langle H - \lambda \widehat{N} \rangle + E_k \left(\sum_{k'} U^\dagger_{kk'} U_{k'k} + V^\dagger_{kk'} V_{k'k} \right) \right] & = & 0 \end{array} \right.$$

$$\sum_{k''} [(h-\lambda)_{k'k''}\, U_{k''k} + \Delta_{k'k''} V_{k''k}] = E_k\, U_{k'k}$$

$$\sum_{k''} \left[(h^*-\lambda)_{k'k''}\, V_{k''k} + \Delta^*_{k'k''} U_{k''k} \right] = -E_k\, V_{k'k}$$

Or

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} \cdot E_k$$

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} \cdot E_k$$

Hartree-Fock Hamiltonian

$$h_{kk'} = t_{kk'} + \Gamma_{kk'}$$

mean-field potential

$$\Gamma_{kk'} = \sum_{qq'} \bar{v}_{kq'k'q}\, \rho_{qq'}$$

pairing potential

$$\Delta_{kk'} = \frac{1}{2} \sum_{qq'} \bar{v}_{kk'qq'}\, \kappa_{qq'}$$

HFB Equations in the coordinate space representation

So far, k, k', k'' can be any basis:

$$\sum_{k''} [(h-\lambda)_{k'k''} U_{k''k} + \Delta_{k'k''} V_{k''k}] \;=\; E_k U_{k'k}$$

$$\sum_{k''} \left[(h^*-\lambda)_{k'k''} V_{k''k} + \Delta^*_{k'k''} U_{k''k}\right] \;=\; -E_k V_{k'k}$$

$$k \to \alpha, \;\; k' \to \boldsymbol{r}, \;\; k'' \to \boldsymbol{r}'$$

$$\int d\boldsymbol{r}' \begin{pmatrix} h(\boldsymbol{r},\boldsymbol{r}') - \lambda & \Delta(\boldsymbol{r},\boldsymbol{r}') \\ -\Delta(\boldsymbol{r},\boldsymbol{r}')^* & -h(\boldsymbol{r},\boldsymbol{r}')^* + \lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}') \\ V_\alpha(\boldsymbol{r}') \end{pmatrix}$$

$$= E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

For a local and zero-range interaction:

$$\langle \boldsymbol{r}_1\boldsymbol{r}_2|v|\boldsymbol{r}_3\boldsymbol{r}_4\rangle = v(\boldsymbol{r}_1)\delta(\boldsymbol{r}_1-\boldsymbol{r}_3)\delta(\boldsymbol{r}_2-\boldsymbol{r}_4)\cdot\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$$

$$\begin{pmatrix} \hat{h}(\boldsymbol{r})-\lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r})^* & -\hat{h}(\boldsymbol{r})+\lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

$$\begin{aligned} \hat{h}(\boldsymbol{r}) &= -\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{HF}}(\boldsymbol{r}), \quad V_{\mathrm{HF}}(\boldsymbol{r}) = v(\boldsymbol{r})\rho(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r}) &= v(\boldsymbol{r})\tilde{\rho}(\boldsymbol{r})/2 \\ \rho(\boldsymbol{r}) &= \sum_\alpha |V_\alpha(\boldsymbol{r})|^2, \quad \tilde{\rho}(\boldsymbol{r}) = -\sum_\alpha U_\alpha(\boldsymbol{r})V_\alpha^*(\boldsymbol{r}) \end{aligned}$$

Ortho-normalization:

$$\int d\boldsymbol{r}\,[U_\alpha^*(\boldsymbol{r})U_{\alpha'}(\boldsymbol{r}) + V_\alpha^*(\boldsymbol{r})V_{\alpha'}(\boldsymbol{r})] = \delta_{\alpha,\alpha'}$$

(note) in condensed matter physics: *Bogoliubov-de Gennes Equations*

(note)

$$\begin{pmatrix} \hat{h}(\boldsymbol{r}) - \lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r})^* & -\hat{h}(\boldsymbol{r}) + \lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

$\Longrightarrow$

$$\begin{pmatrix} \hat{h}(\boldsymbol{r}) - \lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r})^* & -\hat{h}(\boldsymbol{r}) + \lambda \end{pmatrix} \begin{pmatrix} V_\alpha^*(\boldsymbol{r}) \\ U_\alpha^*(\boldsymbol{r}) \end{pmatrix} = -E_\alpha \begin{pmatrix} V_\alpha^*(\boldsymbol{r}) \\ U_\alpha^*(\boldsymbol{r}) \end{pmatrix}$$

We need to consider only one class of solutions.

$\Longrightarrow \quad E_\alpha \geq 0$

Relation to the BCS approximation

$$\begin{pmatrix} \hat{h} - \lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}^*(\boldsymbol{r}) & -\hat{h} + \lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

Expansion on the HF basis:

$$U_\alpha(\boldsymbol{r}) = \sum_i u_i^{(\alpha)} \varphi_i(\boldsymbol{r})$$

$$V_\alpha(\boldsymbol{r}) = \sum_i v_i^{(\alpha)} \varphi_i(\boldsymbol{r})$$

where

$$\hat{h}\varphi_i = \epsilon_i \varphi_i$$

$$\sum_j \begin{pmatrix} (\epsilon_i - \lambda)\delta_{i,j} & \tilde{\Delta}_{ij} \\ \tilde{\Delta}^*_{ij} & (-\epsilon_i + \lambda)\delta_{i,j} \end{pmatrix} \begin{pmatrix} u_j^{(\alpha)} \\ v_j^{(\alpha)} \end{pmatrix} = E_\alpha \begin{pmatrix} u_i^{(\alpha)} \\ v_i^{(\alpha)} \end{pmatrix}$$

diagonalization

$$\tilde{\Delta}_{ij} = \int d\boldsymbol{r}\, \varphi_i^*(\boldsymbol{r}) \tilde{\Delta}(\boldsymbol{r}) \varphi_j(\boldsymbol{r})$$

BCS approximation: Take only the diagonal components in $\tilde{\Delta}_{ij}$

$$
\begin{aligned}
(\epsilon_i - \lambda) u_i^{(\alpha)} + \tilde{\Delta}_{ii} v_i^{(\alpha)} &= E_\alpha u_i^{(\alpha)} \\
\tilde{\Delta}_{ii} u_i^{(\alpha)} + (-\epsilon_i + \lambda) v_i^{(\alpha)} &= E_\alpha v_i^{(\alpha)}
\end{aligned}
$$

Solution:

$$
\begin{aligned}
u_i^{(\alpha)} &= u_\alpha^{\mathrm{BCS}} \delta_{i,\alpha} = \sqrt{\frac{1}{2}\left(1 + \frac{\epsilon_\alpha - \lambda}{E_\alpha}\right)} \\
v_i^{(\alpha)} &= v_\alpha^{\mathrm{BCS}} \delta_{i,\alpha} = \sqrt{\frac{1}{2}\left(1 - \frac{\epsilon_\alpha - \lambda}{E_\alpha}\right)} \\
E_\alpha &= \sqrt{(\epsilon_\alpha - \lambda)^2 + \tilde{\Delta}_{\alpha\alpha}^2}
\end{aligned}
$$

$$
\begin{aligned}
U_\alpha(\boldsymbol{r}) &= u_\alpha^{\mathrm{BCS}} \varphi_\alpha(\boldsymbol{r}) \\
V_\alpha(\boldsymbol{r}) &= v_\alpha^{\mathrm{BCS}} \varphi_\alpha(\boldsymbol{r})
\end{aligned}
$$

$U_\alpha(\boldsymbol{r})$ and $V_\alpha(\boldsymbol{r})$ have the same radial dependence in the BCS approximation.

→ This is not the case in HFB.

Asymptotic Behaviours

$$\begin{pmatrix} \hat{h}(\boldsymbol{r}) - \lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r})^* & -\hat{h}(\boldsymbol{r}) + \lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

$$\boldsymbol{r} \to \infty$$

$$\begin{pmatrix} \hat{T} - \lambda & 0 \\ 0 & -\hat{T} + \lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

Or

$$\left\{ \begin{array}{lcl} \hat{T}\, U_\alpha(\boldsymbol{r}) & = & (E_\alpha + \lambda)\, U_\alpha(\boldsymbol{r}) \\ \hat{T}\, V_\alpha(\boldsymbol{r}) & = & (-E_\alpha + \lambda)\, V_\alpha(\boldsymbol{r}) \end{array} \right.$$

(note) $E_\alpha \geq 0, \quad \lambda < 0$

$$\begin{cases} \hat{T}\,U_\alpha(\boldsymbol{r}) &= (E_\alpha + \lambda)\,U_\alpha(\boldsymbol{r}) \\ \hat{T}\,V_\alpha(\boldsymbol{r}) &= (-E_\alpha + \lambda)\,V_\alpha(\boldsymbol{r}) \end{cases}$$

(note)

$E_\alpha \geq 0, \quad \lambda < 0$

$i)\ 0 \leq E_\alpha \leq -\lambda \longrightarrow E_\alpha + \lambda \leq 0, \quad -E_\alpha + \lambda < 0$

$$U_\alpha(r) \sim e^{-\gamma_u r}, \quad V_\alpha(r) \sim e^{-\gamma_v r}$$

$ii)\ E_\alpha > -\lambda \longrightarrow E_\alpha + \lambda > 0, \quad -E_\alpha + \lambda < 0$

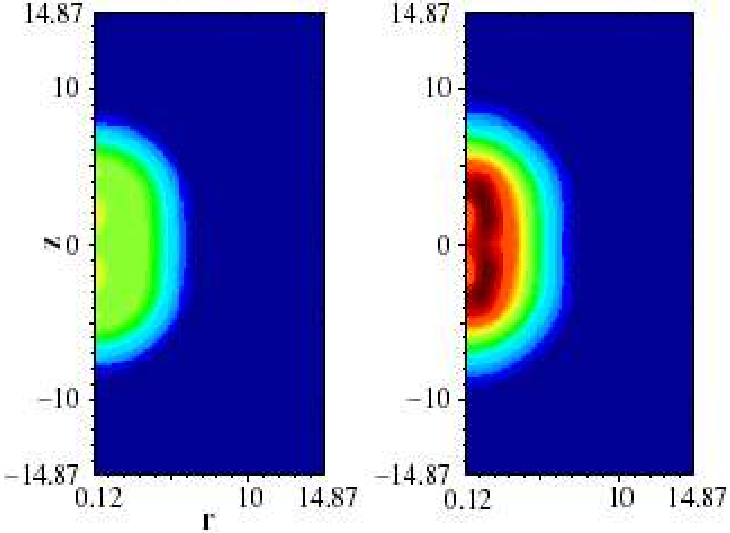
$$\begin{aligned} U_\alpha(r) &\sim \sin(k_u r + \delta + l\pi/2) \\ V_\alpha(r) &\sim e^{-\gamma_v r} \end{aligned}$$

Remarks.

1. $\rho(\boldsymbol{r}) = \sum_\alpha |V_\alpha(\boldsymbol{r})|^2$: always decays exponentially at large distances
2. Deep hole states: appears in the continuum spectra (as very narrow resonance states)

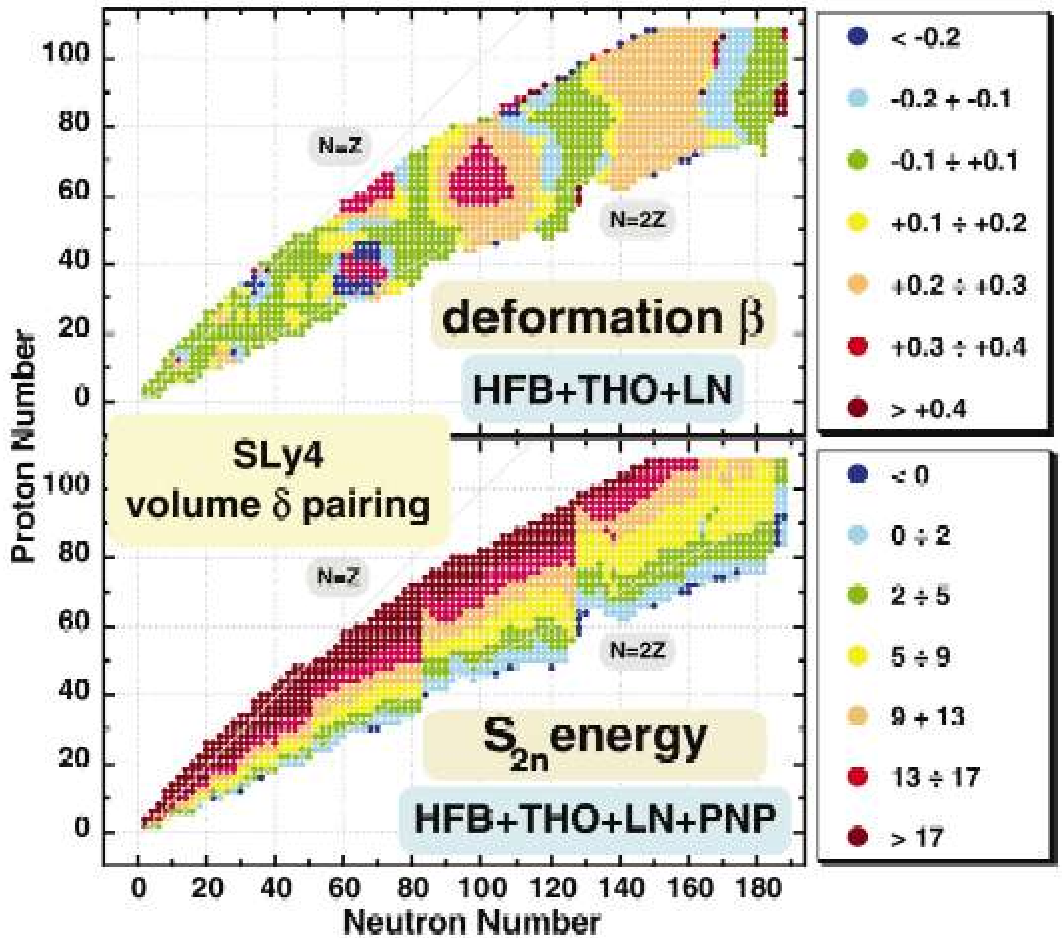
Application of the HFB method

Density of ^{110}Zr (SHFB-SLy4)

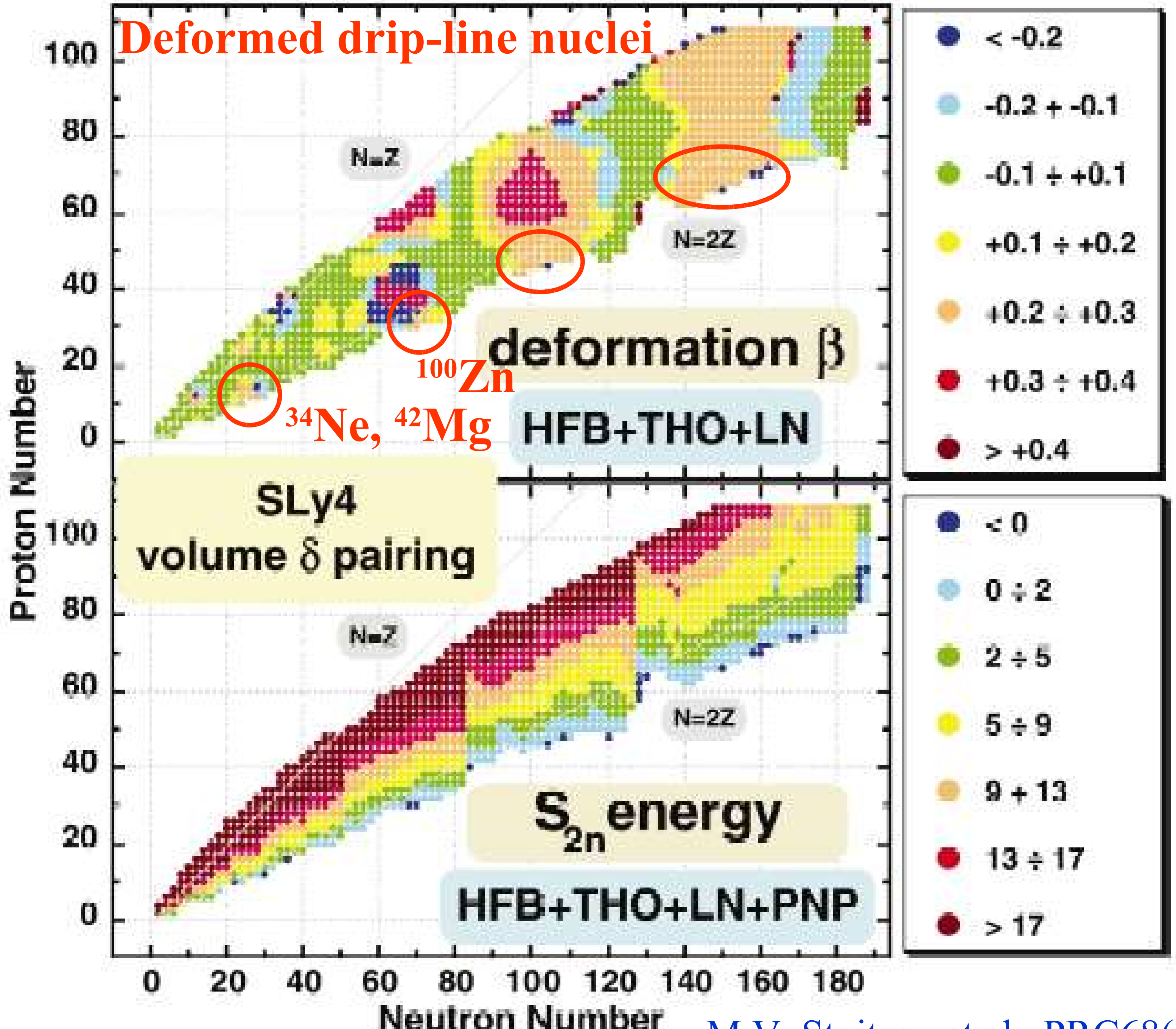


A. Blazkiewicz et al., PRC71('05)054231

Systematics of β_2 and S_{2n}



M.V. Stoitsov et al., PRC68('03)054312

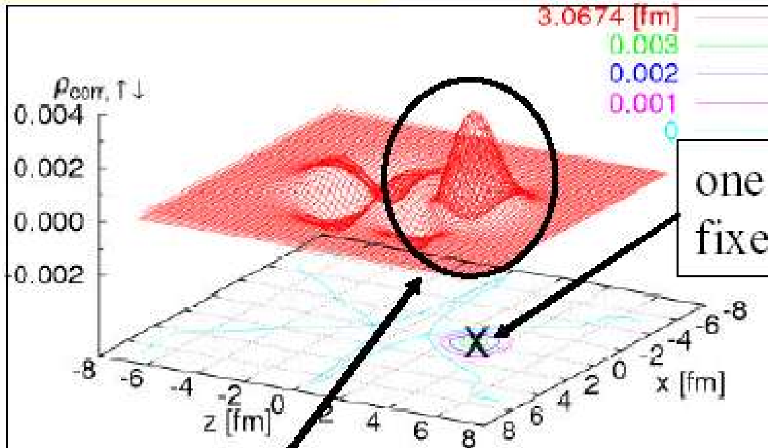


M.V. Stoitsov et al., PRC68('03)054312

Application of the HFB method: di-neutron correlation

Skyrme Ly4
DDDI (mix)

^{22}O



one neutron fixed at $\vec{r}\,'$

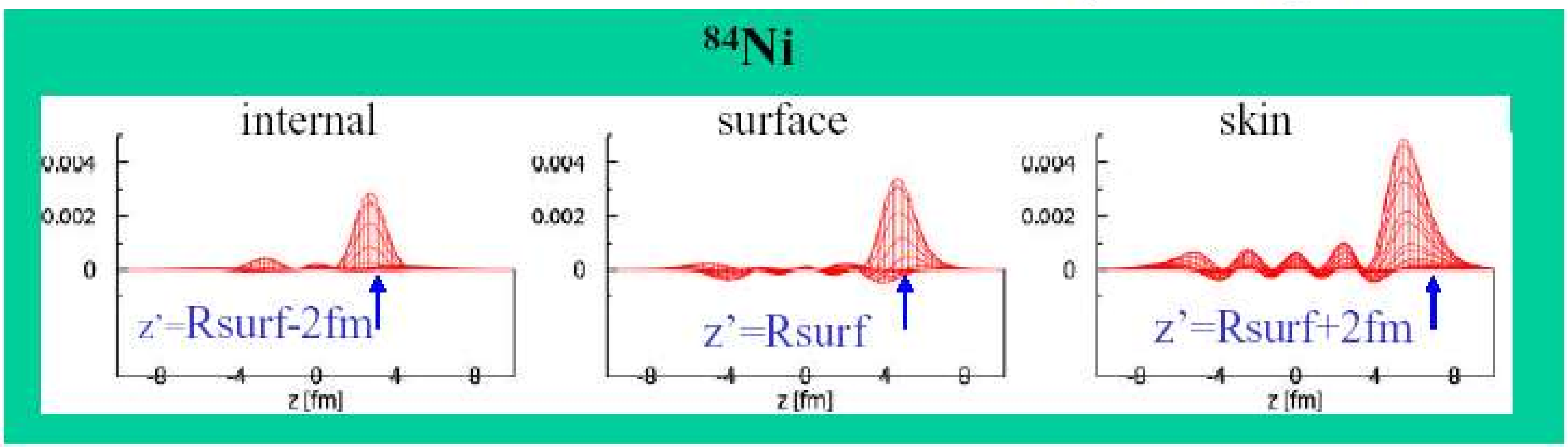
di-neutron correlation

Strongly correlated at short relative distances |r-r'| < 2-3fm

Di-neutron probability

relative weight for $|r-r'|<r_d$

$P(r_d) = 0.27 \quad (r_d=2)$



M. Matsuo, K. Mizuyama, Y. Serizawa, nucl-th/0408052