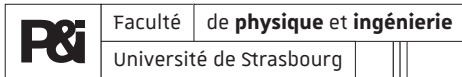


# Study of deformed nuclei around $^{68}\text{Ni}$ in a mean field self-consistent approach

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Supervisor : SIEJA Kamila

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# Table of Contents



- 1 Introduction
- 2 Problematic
- 3 Methodology
- 4 Deformation
- 5 Results
- 6 Conclusions
- 7 Appendix

HF study of  
*Island of  
Inversion*

Introduction

Problematic

Methodology

Deformation

Results

Conclusions

Appendix

# Introduction

Introduction

Problematic

Methodology

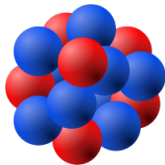
Deformation

Results

Conclusions

Appendix

## Study of nuclei : Proton and Neutron bound state



$$\text{Binding Energy} := \mathbf{BE}(\mathbf{Z}, \mathbf{N}) := (M_{nuclear}(Z, N) - Nm_n - Zm_p)c^2$$

$m_n$  = mass of the neutron  $m_p$  = mass of the proton

# Theory of the Nuclei: a many body problem



HF study of  
*Island of  
Inversion*

Description of nuclei : a theoretical challenge

- Quantum many-body problem ( $A \approx 100$ )

Introduction

Problematic

Methodology

Deformation

Results

Conclusions

Appendix

# Theory of the Nuclei: a many body problem



HF study of  
*Island of  
Inversion*

Description of nuclei : a theoretical challenge

- Quantum many-body problem ( $A \approx 100$ )
- Interaction between nuclei  $\rightarrow$  residues of the interactions between quarks

Introduction

Problematic

Methodology

Deformation

Results

Conclusions

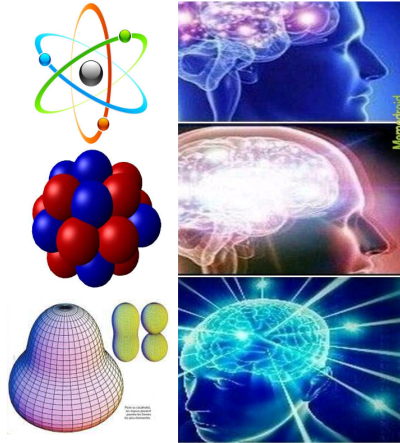
Appendix

# Theory of the Nuclei: a many body problem

Description of nuclei : a theoretical challenge

- Quantum many-body problem ( $A \approx 100$ )
- Interaction between nuclei  $\rightarrow$  residues of the interactions between quarks

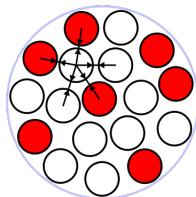
**It needs simplifications**



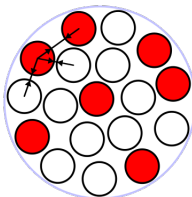
# Macroscopic model : Liquid Drop

Semi-empirical macroscopic model:

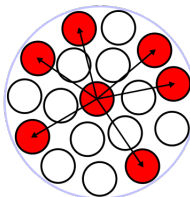
$$BE(Z, N) = a_v A^{1/3} - a_s A^{2/3} - a_c \frac{Z^2 e^2 A^{-1/3}}{4\pi\epsilon_0} - \frac{1}{2} a_a \frac{(N - Z)^2}{A} + \delta(N, Z) \quad (1)$$



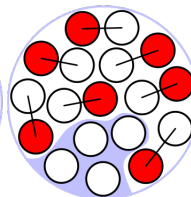
Volume



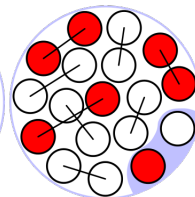
Surface



Coulomb



Asymmetry



Pairing



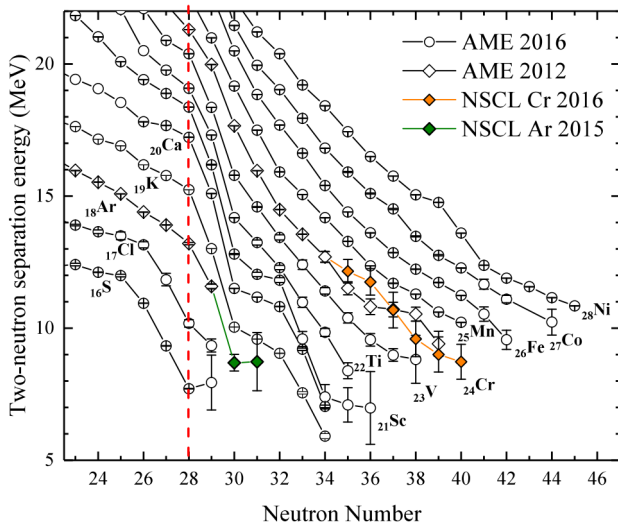
# Two neutron separation

$$S_{2N}(\mathbf{N}, \mathbf{Z}) := \\ BE(Z, N - 2) - BE(Z, N)$$

$$\frac{d}{dN}(S_{2N}) \approx$$

How much less bonded is the new neutron pair with respect to the last one

# Experimental values



Ref[1]



HF study of  
*Island of  
Inversion*

Introduction

Problematic

Methodology

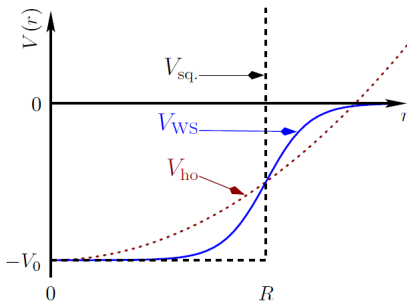
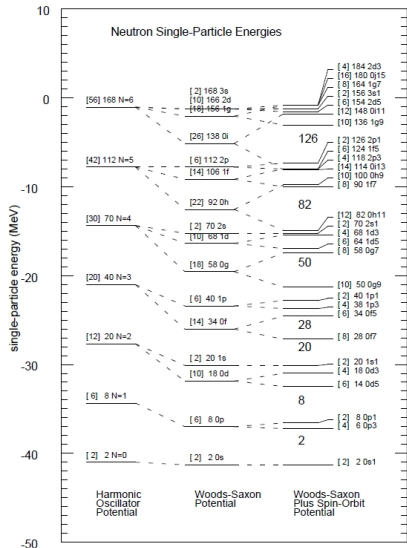
Deformation

Results

Conclusions

Appendix

# Shell Model



- Single particle behaviour in Wood-Saxon potential
- Spin-orbit coupling
- Emergence of all magic numbers

HF study of  
*Island of  
Inversion*

Introduction

Problematic

Methodology

Deformation

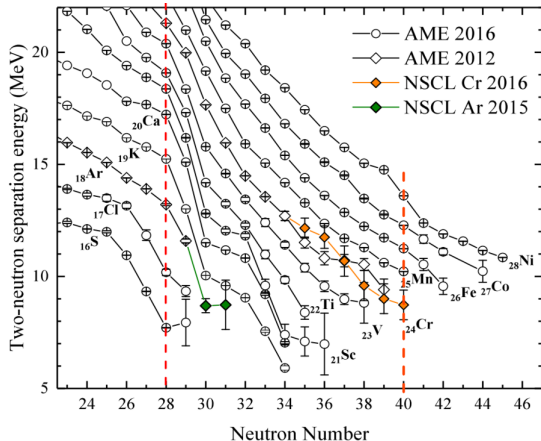
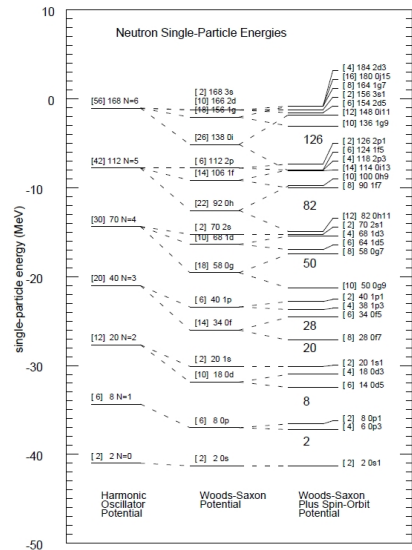
Results

Conclusions

Appendix

# Problematic

# Island of Inversion



HF study of  
*Island of  
Inversion*

Introduction

Problematic

Methodology

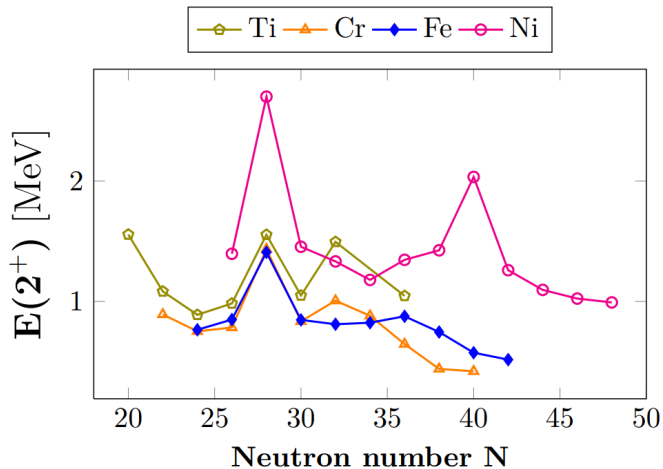
Deformation

Results

Conclusions

Appendix

# Other experimental evidence



Ref [2]

# Methodology

# Hartree-Fock Method



HF study of  
*Island of  
Inversion*

Variational principle:

$\{\phi_\alpha(\vec{r})\}$  form a Slater determinant

$$\forall \phi_i^*(\vec{r}) \in \{\phi_\alpha^*(\vec{r})\} : \\ \frac{\partial}{\partial \phi_i^*(\vec{r})} \{E(C) - \sum_\alpha \epsilon_\alpha \int d\tau_1 |\phi_\alpha(\vec{r}_1)|^2\} = 0$$

Mean field equations:

$$T\phi_i(\vec{r}) + \left\{ \sum_\alpha \int d\tau_1 \phi_\alpha^*(\vec{r}_1) V(\vec{r}\vec{r}_1) \phi_\alpha(\vec{r}_1) \right\} \phi_i(\vec{r}) \\ - \int d\tau_1 \left\{ \sum_\alpha \phi_\alpha^*(\vec{r}_1) V(\vec{r}\vec{r}_1) \phi_\alpha(\vec{r}) \right\} \phi_i(\vec{r}_1) = \epsilon_i \phi_i(\vec{r})$$

Introduction

Problematic

Methodology

Deformation

Results

Conclusions

Appendix



# Hartree Fock Method

$$\begin{array}{c}
 \{\phi_\alpha^*(\vec{r})\} \xrightarrow{\hspace{10em}} T\phi_i(\vec{r}) + \left\{ \sum_\alpha \int d\tau_1 \phi_\alpha^*(\vec{r}_1) V(\vec{r}\vec{r}_1) \phi_\alpha(\vec{r}_1) \right\} \phi_i(\vec{r}) \\
 \uparrow \\
 \{\phi_i^*(\vec{r})\} \\
 \uparrow \\
 H_{HF}\phi_i(\vec{r}_1) = \epsilon_i\phi_i(\vec{r}) \leftarrow T\phi_i(\vec{r}_1) + V_{HF}\phi_i(\vec{r}_1) = H_{HF}\phi_i(\vec{r}_1) \\
 \downarrow \\
 - \int d\tau_1 \left\{ \sum_\alpha \phi_\alpha^*(\vec{r}_1) V(\vec{r}\vec{r}_1) \phi_\alpha(\vec{r}) \right\} \phi_i(\vec{r}_1) = \epsilon_i\phi_i(\vec{r})
 \end{array}$$

Modelisation of the two body interaction :

$$\begin{aligned} V_{sky}(1, 2) = & \quad t_0(1 + x_0 P^\sigma) \delta(\vec{r}_1 - \vec{r}_2) \\ + & \quad \frac{1}{2} t_1(1 + x_1 P^\sigma) [\delta(\vec{r}_1 - \vec{r}_2) \mathbf{k}^2 + \mathbf{k}'^2 \delta(\vec{r}_1 - \vec{r}_2)] \\ + & \quad t_2(1 + x_2 P^\sigma) \mathbf{k}' \delta(r_{12}) \mathbf{k} \\ + & \quad i W_0 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \mathbf{k}' \times \delta(\vec{r}_1 - \vec{r}_2) \mathbf{k} \\ + & \quad \frac{1}{6} t_3(1 + x_3 P^\sigma) \rho^{\gamma_{00}} \left( \frac{r_1 + r_2}{2} \right) \delta(\vec{r}_1 - \vec{r}_2) \end{aligned}$$

# BCS Theory (BARDEEN, COOPER, SCHRIEFFER)

Interaction :

- pair coupling
- short range
- between particles of equal in norm and opposed spin

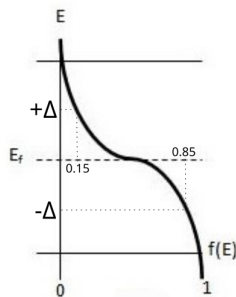


Figure:  $\Delta$  = Pairing gap

$E$  = single particle energy

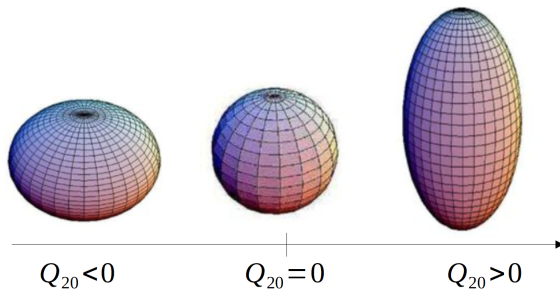
$E_f$  = Fermi level

$f(E)$  = single particle level occupation

# Deformation

# deformation of the nuclei

- Wood-Saxon + spin-orbit : spherical solutions
- Hartree-Fock + Skyrme + BCS : Allow deformed nuclei



$$\hat{Q}_{20} = \sqrt{\frac{16\pi}{5}} (2\hat{z}^2 - \hat{x}^2 - \hat{y}^2) \quad \beta_p = \frac{\sqrt{5\pi}}{3} \frac{Q_{20}(\rho_e)}{ZeR_0^2}$$

# Results

# Process



HF study of  
*Island of  
Inversion*

Introduction

Problematic

Methodology

Deformation

Results

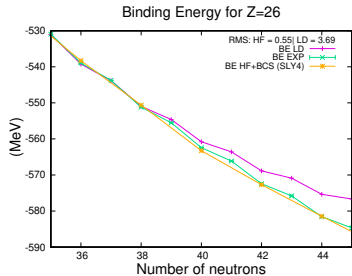
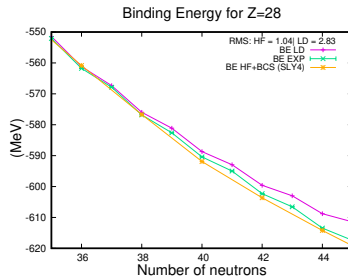
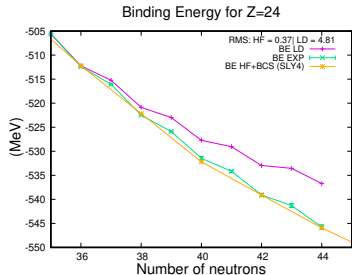
Conclusions

Appendix

```
1 is file contains the input data for htda code.
2 The informations are found by using a "keyword" in the line preceding the one
3 where these info. are given. These keywords are:
4 =====
5 Nuclid: N Z
6 48 28
7 -----
8 Skyrme force type: (1:SIII, 2:SKM*, 3:SLY4)
9 3
10 -----
11 Truncated basis: N0(major shells) B0(oscillator para.) Q(deformation para.)
12 12 0.5000 1.150
13 Degree of Gauss integration methods: Hermite Laguerre
14 50 16
15 Maximum numbers of iterations of the type: HF<=1000, HTDA<=1000, BCS<=1000
16 100 0 100
17 Deformation constraints: (C1 Q2(barn) C4 Q4 (barn^2))
18 0.000 0.000
19 0.000 000
20 -----
21 BCS parameter
22 *Pairing force (G0)(neutrons, protons) and truncation BCS parameter (MeV)
23 16.1 13.3
24 65D-1
25 -----
26 HTDA parameters:
27 *Delta force: (neutrons protons np1 np0)
28 -300D0 -300D0 -300d0 -600d0
29 *Excitation Window
30 65D-1
31 *Fenetre REDUITE (Delta E, Cut-off in energy, Weight-function's X and mu,)
32 65D-1 1000
33 65D-1 0.2
```

```
34 *Many-body matrix element diagonalisation (EIDEN, EPHTDA)
35 1D0 1D-25
36 *Residual interaction
37 0
38 *K/pi
39 0 1 0 1
40 -----
41 Mixing parameter (HF,HTDA)
42 4D-1 5D-1
43 -----
44 Options
45 *Initial potential from (0: Calcul(Woods-Saxon), 1: file HFfields.in)
46 0
47 *Limitations for one pair transfers
48 1
49 *Matrix calculation (0: do, 1: don't)
50 0
51 *PN coupling included (0: not, 1: do)
52 0
53 -----
54 Converged condition
55 5D-6 1D-2 1D-2
56 -----
57 Do simplex (1: Yes, 0: No)
58 0
59 -----
60 * eigenvalues, Lanczos precision, Lanczos iteration number, file for vectors
```

# Binding Energy



RMS (in MeV) for the different Skyrme forces:

Z	SIII	SKM*	SLY4	LD
24	2.40	6.58	0.37	4.81
26	2.72	4.60	0.55	3.69
28	2.60	3.15	1.04	2.83

HF study of  
*Island of  
Inversion*

Introduction

Problematic

Methodology

Deformation

Results

Conclusions

Appendix



# two neutron separation



HF study of  
*Island of  
Inversion*

Introduction

Problematic

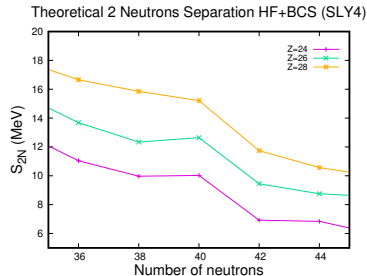
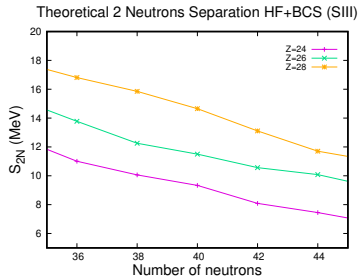
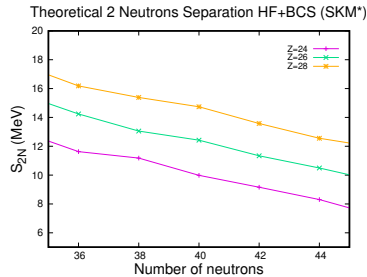
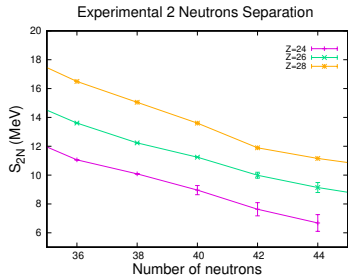
Methodology

Deformation

Results

Conclusions

Appendix

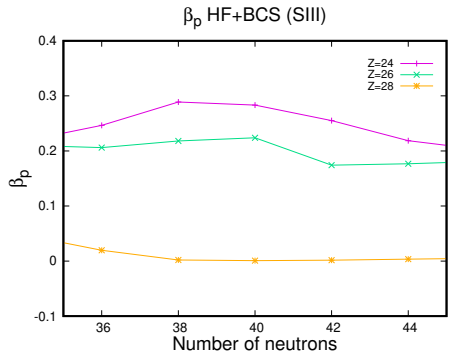
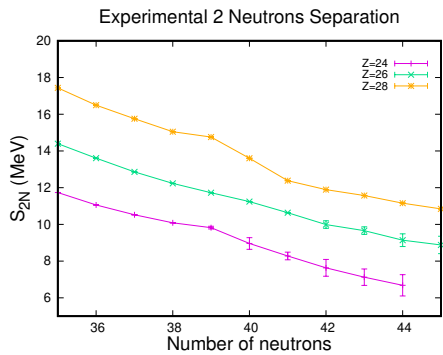


# deformation

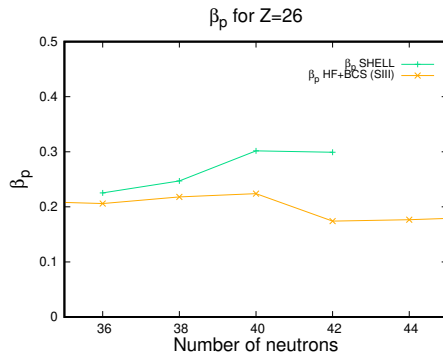
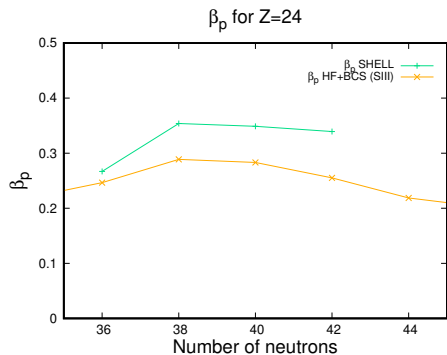


HF study of  
*Island of  
Inversion*

- Introduction
- Problematic
- Methodology
- Deformation
- Results**
- Conclusions
- Appendix

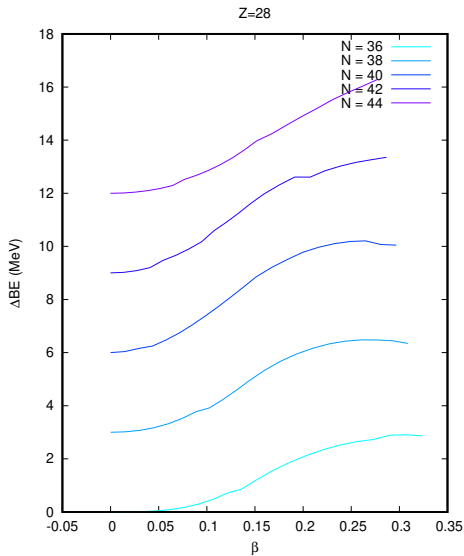
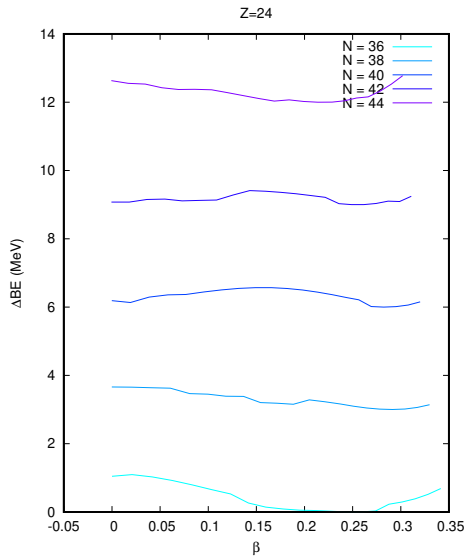


# comparison with other calculations



*SHELL* : Ref [3]

# constrained calculations (SIII)



# Conclusions

- **Problematic :**

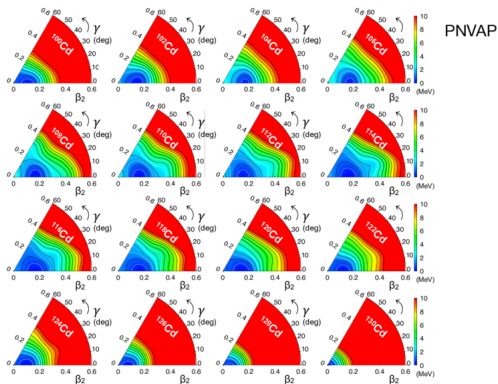
- Liquid drop and shell models struggles in some area of the nuclear chart
- Island of inversion around  $^{68}\text{Ni}$

- **What we did :**

- Study Cr,Fe and Ni around N=40 using Hartree-Fock calculations
- Creation of an environment in C++ in order to produce results

- **What we found :**

- Some features of the Cr,Fe and Ni isotopes lines can be explained with predicted deformations
- Predicted sphericity of Ni points toward double magicity of  $^{68}\text{Ni}$



**Figure:** (Color online) PNVAP potential energy surfaces as a function of the  $(\beta_2, \gamma)$  deformation parameters for the even-mass 100-130 Cd isotopes. The results are obtained with the Gogny-D1S interaction within the SCCM approach.

# References I

- [1] M. Mougeot, “Nuclear Collectivity Studied through High-precision Mass Measurements of Neutron-rich Argon and Chromium Isotopes,” Jan 2019. Presented 30 Nov 2018.
- [2] S. Naimi, *Onsets of nuclear deformation from measurements with the ISOLTRAP mass spectrometer*. Theses, Université Paris-Diderot - Paris VII, Oct. 2010.
- [3] S. M. Lenzi, F. Nowacki, A. Poves, and K. Sieja, “Island of inversion around  $^{64}\text{Cr}$ ,” *Phys. Rev. C*, vol. 82, p. 054301, Nov 2010.
- [4] D. of Education Open Textbook Pilot Project, “Fermi energy and fermi surface,” 2021.
- [5] Wikipedia, “Semi-empirical-mass-formula,” 2022.



## References II

- [6] A. A. Al-Sammarraie, “Potentials radial dependence, square well v sq ., harmonic oscillator v ho , and woods-saxon potential v ws,” 2022.
- [7] M. Hjorth-Jensen, “Course2manybodymethods,” 2015.
- [8] O. Delaune, *Technique de la cinématique inverse pour l'étude des rendements isotopiques des fragments de fission aux énergies GANIL*. Theses, Université de Caen, Oct. 2012.
- [9] M. Siciliano, J. Valiente-Dobón, A. Goasduff, T. Rodríguez, D. Bazzacco, G. Benzoni, T. Braunroth, N. Cieplicka-Oryńczak, E. Clement, F. Crespi, G. de France, M. Doncel, S. Erturk, C. Fransen, A. Gadea, G. Georgiev, A. Goldkuhle, U. Jakobsson, G. Jaworski, and D. Testov, “Lifetime measurements in the even-even  $^{102-108}\text{Cd}$  isotopes,” 01 2021.

# Appendix

$$\begin{aligned} V_{sky}(1, 2) = & t_0(1 + x_0 P^\sigma) \delta(r_1 - r_2) \\ & + \frac{1}{2} t_1(1 + x_1 P^\sigma) [\delta(r_1 - r_2) \mathbf{k}^2 + \mathbf{k}'^2 \delta(r_1 - r_2)] \\ & + t_2(1 + x_2 P^\sigma) \mathbf{k}' \delta(r_{12}) \mathbf{k} \\ & + iW_0(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \mathbf{k}' \times \delta(r_1 - r_2) \mathbf{k} \\ & + \frac{1}{6} t_3(1 + x_3 P^\sigma) \rho^{\gamma_{00}}(\frac{r_1+r_2}{2}) \delta(r_1 - r_2) \end{aligned}$$

$$\mathbf{k} = \frac{1}{2i}(\vec{\nabla}_1 - \vec{\nabla}_2) ; \mathbf{k}' = \mathbf{k} \text{ acting on the left ; } P^\sigma = \frac{1}{2}(1 + \vec{\sigma}_1 \vec{\sigma}_2)$$

# Skyrme parameters

	SIII [4]	SkM* [21]	SLy4 [22]
$t_0$	-1128	75	-2645
$t_1$	395	0	410
$t_2$	-95	0	-135
$t_3$	14000	0	15595
$x_0$	0	45	0
$x_1$	0	0	0
$x_2$	0	0	0
$x_3$	1	0	0
$\gamma$	1	0	1
$W_0$	130	0	120

Introduction

Problematic

Methodology

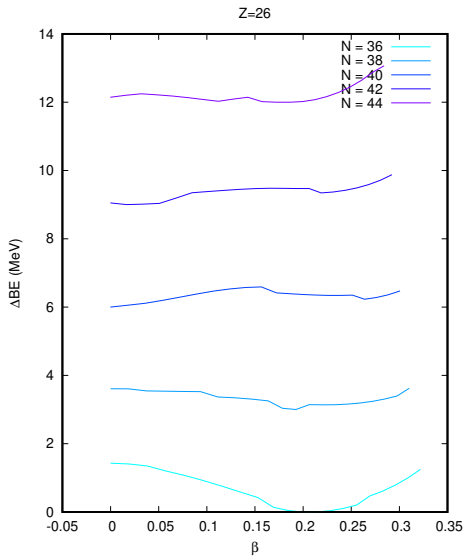
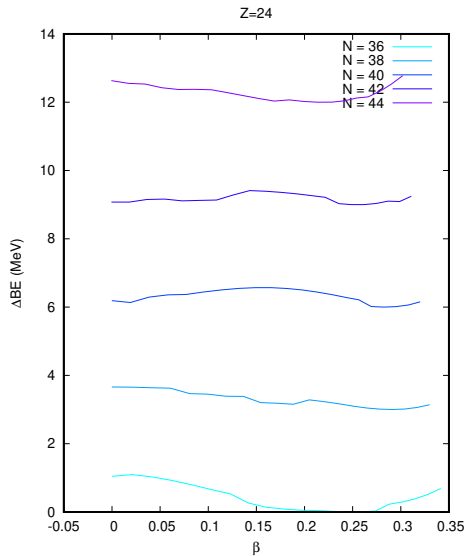
Deformation

Results

Conclusions

Appendix

# constrained calculations (SIII)



# BCS equation

$$\hat{H} = \sum_{\nu} e_{\nu} a_{\nu}^{\dagger} a_{\nu} - G \sum_{\nu > 0, \nu' > 0} a_{\nu}^{\dagger} a_{-\nu}^{\dagger} a_{-\nu'} a_{\nu'}$$

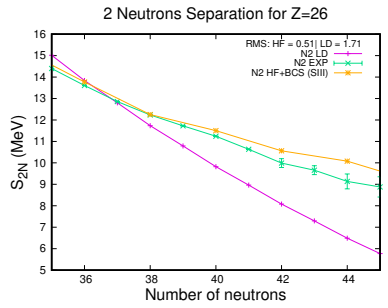
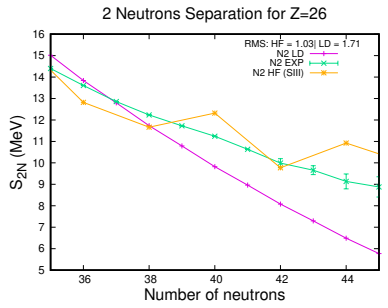


Figure: Comparison: without BCS (left);with BCS (right)