

Mean field developments: formalism and interactions

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Shell model- Mean field connection

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Intrinsic vs Laboratory Frame Description of the Deformed Nucleus ^{48}Cr

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The collective yrast band of the nucleus ^{48}Cr is studied using the spherical shell model and the Hartree-Fock-Bogoliubov (HFB) method. Both approaches produce basically the same axially symmetric intrinsic state up to the—accurately reproduced—observed backbending. Agreement between both calculations extends to most observables. The only significant discrepancy comes from the static moments of inertia and can be attributed to the need of a more refined treatment of pairing correlations in the HFB calculation.

Appart from the good agreement with experiment, the connection was made through the "spherical shell occupancies"

$$\nu(nlj) = \sum_m \langle \Phi | c_{nljm}^+ c_{nljm} | \Phi \rangle$$

that turned out to be essentially the same in both approaches.

The mean field approach

The mean field aims at a reproduction of bulk nuclear properties over the whole Nuclide chart within an **independent particle** framework

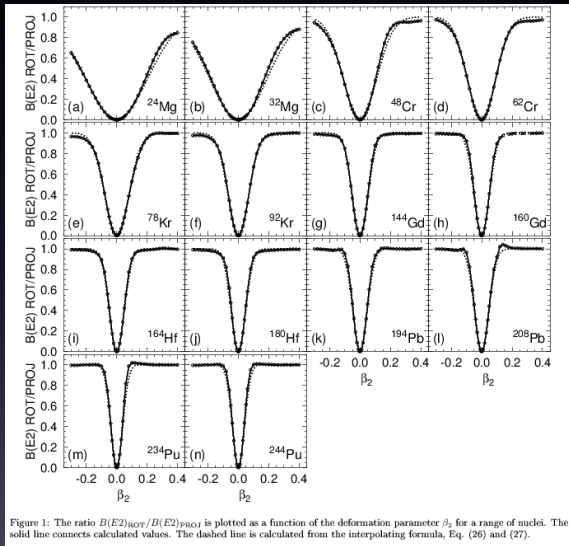
- Spontaneous symmetry breaking (HFB, deformation)
- Effective phenomenological interactions

Successful mass tables have been created (Gogny D1M, HFB-17, Relativistic DD coupling models) and a lot of phenomenology is described (moments of inertia, fission barrier heights, low energy spectroscopy, etc)

Missing correlations are important for a high-quality description of data

- Symmetry restoration (good quantum numbers)
- Configuration mixing (coexistence and spectroscopy)

A couple of examples



Validity of rotational formula for $B(E2)$ and weakly def nuclei

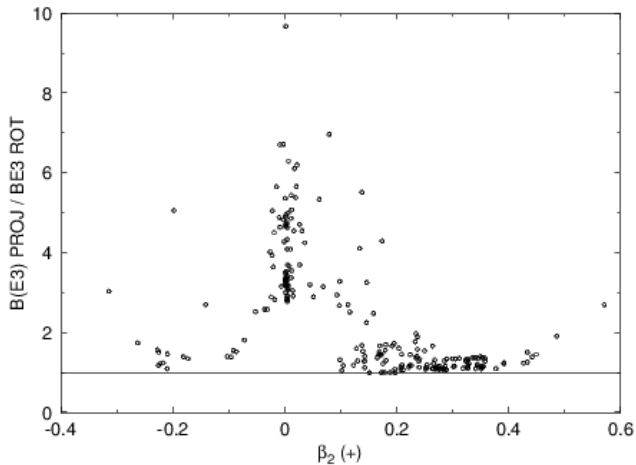


Figure 5: The ratio $B(E3, 3^- \rightarrow 0^+)_{\text{PROJ}} / B(E3, 3^- \rightarrow 0^+)_{\text{ROT}}$ is plotted as a function of the $\beta_2(+)$ quadrupole deformation parameter of the positive parity intrinsic state.

Outline

We will focus today in two aspects of the mean field approximation

- 1 Pfaffians: evaluation of overlaps between HFB wave functions

Configuration mixing

Symmetry restoration

Onishi formula and the Generalized Wick Theorem

- *Sign problem*
- *Combinatorial explosion*
- *Different bases*

- 2 BCPM: An alternative to Skyrme and Gogny

- based on realistic microscopic nuclear matter EOS
- Fitted to spherical and deformed even-even nuclei
- Few, easy to understand, parameters

Collaborators: G. F. Bertsch; M. Baldo, P. Schuck and X. Viñas

Configuration mixing: GCM

GCM wf are linear combinations of HFB states

$$|\Psi\rangle = \int dQ f(Q) |\phi(Q)\rangle + \sum \int dQ f_{ij}(Q) \beta_i^+ \beta_j^+ |\phi(Q)\rangle \dots$$

Amplitudes f , f_{ij} , etc from variational principle

Overlaps required

- $\langle \phi | \phi' \rangle$
- $\langle \phi | \hat{O} | \phi' \rangle$
- $\langle \phi | \beta_1 \dots \beta_r \bar{\beta}_1^+ \dots \bar{\beta}_s^+ | \phi' \rangle$
- $\langle \phi | \beta_1 \dots \beta_r \hat{O} \bar{\beta}_1^+ \dots \bar{\beta}_s^+ | \phi' \rangle$

$|\phi\rangle$ and $|\phi'\rangle$ are HFB wave functions

Symmetry breaking and restoration

- Nuclear superfluidity (Particle number, BCS like w.f.)
- Rotational bands (Rotational symmetry)
- Octupole bands (Parity)
- Translational invariance

PNP as an example

$$|\Psi^N\rangle = \hat{P}^N |\Phi\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi(\hat{N}-N)} |\Phi\rangle$$

- $\langle\Phi|e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$
- $\langle\Phi|\hat{O}e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$
- $\langle\Phi|\beta_1 \dots \beta_r \bar{\beta}_1^+ \dots \bar{\beta}_s^+ e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$
- $\langle\Phi|\beta_1 \dots \beta_r \hat{O} \bar{\beta}_1^+ \dots \bar{\beta}_s^+ e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$

$e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$ is a HFB wave function (Thouless theorem)

Tools: Onishi formula and GWT

Onishi formula

$$\langle \phi | \phi' \rangle = \pm \sqrt{\det(U^+ U' + V^+ V')}$$

sign undefined !

Operator and multiquasiparticle overlaps use the Generalized Wick Theorem (Balian and Brezin, Hara, Gaudin, ...)

$$\frac{\langle \phi | \beta_1 \dots \beta_r \bar{\beta}_1^+ \bar{\beta}_s^+ | \phi' \rangle}{\langle \phi | \phi' \rangle} = \sum \text{Contractions}$$

Contractions

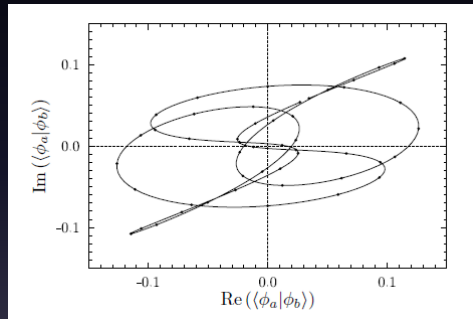
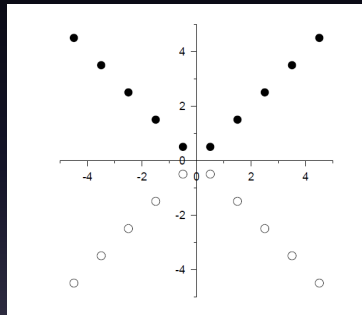
$$\frac{\langle \phi | \beta_\mu \beta_\nu | \phi' \rangle}{\langle \phi | \phi' \rangle} \quad \frac{\langle \phi | \bar{\beta}_\sigma^+ \bar{\beta}_\tau^+ | \phi' \rangle}{\langle \phi | \phi' \rangle} \quad \frac{\langle \phi | \beta_\mu \bar{\beta}_\tau^+ | \phi' \rangle}{\langle \phi | \phi' \rangle}$$

Combinatorial explosion: $(r + s - 1)!!$ terms (11 !! = 10395)

Sign of HFB overlaps

The sign of $\langle \phi | \phi' \rangle$ is undefined (square root)

Overlaps computed on a discrete mesh and used in sums



Of the order of 10^8-10^{10} overlaps required in typical calculations for a single nucleus. Large variety of nuclei (spherical, deformed, ...) call for a robust determination of the sign.

New formula to evaluate the overlap ¹

The formula relies on the powerful concept of Fermion Coherent States $|\mathbf{z}\rangle$ parametrized in terms of the anti-commuting elements z_k and z_k^* of a **Grassmann algebra** and given by the conditions

$$a_k|\mathbf{z}\rangle = z_k|\mathbf{z}\rangle$$

and

$$\langle\mathbf{z}|a_k^+ = z_k^*\langle\mathbf{z}|$$

The coherent states satisfy a closure relation

$$1 = \int d\mu(\mathbf{z})|\mathbf{z}\rangle\langle\mathbf{z}|$$

¹ *Sign of the overlap of Hartree-Fock-Bogoliubov wave functions*, L.M. Robledo, Phys Rev C 79, 021302(R) (2009)

Introducing the HFB wave functions in the Thouless parametrization

$$|\phi_i\rangle = \exp\left(\frac{1}{2} \sum_{kk'} M_{kk'}^{(i)} a_k^+ a_{k'}^+\right) |0\rangle$$

with the skew-symmetric $M^{(i)} = (V_i U_i^{-1})^*$ the evaluation of the overlap is carried out by introducing the closure relation

$$\langle\phi_0|\phi_1\rangle = \int d\mu(\mathbf{z}) \langle 0 | e^{\frac{1}{2} \sum_{kk'} M_{kk'}^{(0)*} a_{k'} a_k} | \mathbf{z} \rangle \langle \mathbf{z} | e^{\frac{1}{2} \sum_{kk'} M_{kk'}^{(1)} a_k^+ a_{k'}^+} | 0 \rangle$$

and using the properties of $|\mathbf{z}\rangle$

$$e^{\frac{1}{2} \sum_{kk'} M_{kk'}^{(0)*} a_{k'} a_k} | \mathbf{z} \rangle = e^{\frac{1}{2} \sum_{kk'} M_{kk'}^{(0)*} z_{k'} z_k} | \mathbf{z} \rangle$$

$$\langle \phi_0 | \phi_1 \rangle = \int d\mu(\mathbf{z}) e^{\frac{1}{2} \sum_{kk'} M_{kk'}^{(0)*} z_{k'} z_k} e^{\frac{1}{2} \sum_{kk'} M_{kk'}^{(1)} z_k^* z_{k'}^*}$$

Introducing

$$\mathbb{M}_{\mu'\mu} = \begin{pmatrix} M_{k'k}^{(1)} & -\mathbf{1}_{k'k} \\ \mathbf{1}_{k'k} & -M_{k'k}^{(0)*} \end{pmatrix}$$

and $z_\mu = (z_{k'}^*, z_{k'})$ then

$$\langle \phi_0 | \phi_1 \rangle = \int \prod_k (dz_k^* dz_k) e^{\frac{1}{2} \sum_{\mu\mu'} z_{\mu'} \mathbb{M}_{\mu'\mu} z_\mu}$$

which is a Gaussian integral well known in QFT.

$$\langle \phi_0 | \phi_1 \rangle = s_N \text{Pf}(\mathbb{M}) = s_N \text{Pf} \begin{pmatrix} M^{(1)} & -\mathbf{1} \\ \mathbf{1} & -M^{(0)*} \end{pmatrix}$$

where $s_N = (-1)^{N(N+1)/2}$

Pfaffian

$\text{pf}A$ is the Pfaffian of the skew-symmetric matrix A .

- It is similar to the determinant

for a 2×2 matrix $R = \begin{pmatrix} 0 & r_{12} \\ -r_{12} & 0 \end{pmatrix}$ we obtain $\text{pf}(R) = r_{12}$

for a 4×4 matrix $R = \begin{pmatrix} 0 & r_{12} & r_{13} & r_{14} \\ -r_{12} & 0 & r_{23} & r_{24} \\ -r_{13} & -r_{23} & 0 & r_{34} \\ -r_{14} & -r_{24} & -r_{34} & 0 \end{pmatrix}$

$$\text{pf}(R) = r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}$$

- $\text{pf}(T^t R T) = \det(T) \text{pf}(R)$
- Minor-like expansion formula
- $\text{pf}(R) = \sqrt{\det(R)}$

Numerical evaluation

- Straightforward using Householder (orthogonal) transformations to bring the matrix in tridiagonal form

$$\text{pf} \begin{pmatrix} 0 & r_{12} & 0 & 0 \\ -r_{12} & 0 & r_{23} & 0 \\ 0 & -r_{23} & 0 & r_{34} \\ 0 & 0 & -r_{34} & 0 \end{pmatrix} = r_{12}r_{34}$$

- Aitken's block diagonalization formula can be used

$$\begin{pmatrix} \mathbb{I} & 0 \\ Q^T R^{-1} & \mathbb{I} \end{pmatrix} \begin{pmatrix} R & Q \\ -Q^T & S \end{pmatrix} \begin{pmatrix} \mathbb{I} & -R^{-1}Q \\ 0 & \mathbb{I} \end{pmatrix} = \begin{pmatrix} R & 0 \\ 0 & S + Q^T R^{-1}Q \end{pmatrix} \quad (1)$$

- FORTRAN, Mathematica and Python routines available at CPC Software Library

The advantages of the present approach are

- Calculation of eigenvalues avoided
- Can be extended to the evaluation of traces of density matrix operators (finite temperature).
- Performing algorithms for the numerical evaluation of the Pfaffian exist.
- Fully occupied levels ($\nu=1$) can be easily handled to avoid in a very clean way the indeterminacy that appear in this case^(*)
- Empty levels ($\nu=0$) can also be handled reducing computational burden even more^(*)

^(*) L.M.Robledo, Phys Rev C84, 014307 (2011)

Another derivation

Note that

$$\langle |\beta_1 \beta_2 \bar{\beta}_3 \bar{\beta}_4| \rangle = r_{12} r_{34} - r_{13} r_{24} + r_{14} r_{23}$$

where r_{ij} are the contractions

$$\text{pf} \begin{pmatrix} 0 & r_{12} & r_{13} & r_{14} \\ -r_{12} & 0 & r_{23} & r_{24} \\ -r_{13} & -r_{23} & 0 & r_{34} \\ -r_{14} & -r_{24} & -r_{34} & 0 \end{pmatrix} = r_{12} r_{34} - r_{13} r_{24} + r_{14} r_{23}$$

from here

$$\langle |\beta_1 \dots \beta_P \bar{\beta}_1 \dots \bar{\beta}_Q| \rangle = \text{pf}(\mathbf{S}_{ij})$$

where \mathbf{S}_{ij} is the skew symmetric $(P + Q) \times (P + Q)$ matrix such that \mathbf{S}_{ij} $i < j$ are the possible contractions

$$\langle |\beta_k \beta_l| \rangle \quad \langle |\beta_k \bar{\beta}_r| \rangle \quad \langle |\bar{\beta}_r \bar{\beta}_s| \rangle$$

$$\langle \tilde{\phi} | \tilde{\phi}' \rangle = \langle |\beta_{2n} \dots \beta_1 \beta_1^{\prime+} \dots \beta_{2n}^{\prime+}| \rangle = (-1)^n \text{pf} \mathbf{S}$$

Contractions

$$\langle |\beta_\mu \beta_\nu| \rangle = \mathbf{V}^T \mathbf{U} \quad \langle |\beta_\mu \beta_\nu^{\prime+}| \rangle = \mathbf{V}^T \mathbf{V}'^* \quad \langle |\beta_\mu^{\prime+} \beta_\nu^{\prime+}| \rangle = \mathbf{U}'^+ \mathbf{V}'^*$$

$$\langle \tilde{\phi} | \tilde{\phi}' \rangle = (-1)^n \text{pf} \begin{bmatrix} \mathbf{V}^T \mathbf{U} & \mathbf{V}^T \mathbf{V}'^* \\ -\mathbf{V}'^\dagger \mathbf{V} & \mathbf{U}'^\dagger \mathbf{V}'^* \end{bmatrix}$$

\mathcal{R} a symmetry operator

$$\langle \tilde{\phi} | \mathcal{R} | \tilde{\phi}' \rangle = (-1)^n \text{pf} \begin{bmatrix} \mathbf{V}^T \mathbf{U} & \mathbf{V}^T \mathbf{R}^T \mathbf{V}'^* \\ -\mathbf{V}'^\dagger \mathbf{R} \mathbf{V} & \mathbf{U}'^\dagger \mathbf{V}'^* \end{bmatrix}$$

R is the matrix of matrix elements of \mathcal{R}

Most general multi-quasiparticle overlap

$$\langle \phi | \bar{\beta}_{\mu_r} \cdots \bar{\beta}_{\mu_1} \mathcal{R} \bar{\beta}'_{\nu_1} \cdots \bar{\beta}'_{\nu_s} | \phi' \rangle = (-1)^n (-1)^{r(r-1)/2} \frac{\det C^* \det C'}{\prod_{\alpha}^n v_{\alpha}^* v'_{\alpha}}$$

$$\times \text{pf} \begin{bmatrix} V^T U & V^T \mathbf{p}^{\dagger} & V^T R^T \mathbf{q}'^T & V^T R^T V'^* \\ -\mathbf{p}^* V & \mathbf{q}^* \mathbf{p}^{\dagger} & \mathbf{q}^* R^T \mathbf{q}'^T & \mathbf{q}^* R^T V'^* \\ -\mathbf{q}' R V & -\mathbf{q}' R \mathbf{q}^{\dagger} & \mathbf{p}' \mathbf{q}'^T & \mathbf{p}' V'^* \\ -V'^{\dagger} R V & -V'^{\dagger} R \mathbf{q}^{\dagger} & -V'^{\dagger} \mathbf{p}'^T & U'^{\dagger} V'^* \end{bmatrix}.$$

$$\mathbf{p}_{\mu_j m} = \bar{V}_{m\mu_j} \quad (\text{dimension } r \times 2n)$$

$$\mathbf{q}_{\mu_j m} = \bar{U}_{m\mu_j} \quad (\text{dimension } s \times 2n)$$

Valid for "blocked HFB states" (odd-A nuclei)

Avoids combinatorial explosion !

$\langle \phi | \beta_1 \beta_2 \beta_3 \hat{H} \beta'_4 \beta'_5 \beta'_6 | \phi' \rangle$ is the energy of 1p-1h excitations in odd-A nuclei. It involves $9!! = 945$ terms

Different bases

Very often the quasiparticle operators of $|\phi\rangle$ and $|\phi'\rangle$ are defined in terms of different single particle bases that do not span the same Hilbert subspace

- Translated
- Rotated
- Different oscillator lengths

Previous formulas assume equal bases

Solution: Simply take \mathcal{R} as the operator transforming one basis into another (non unitary in general). R becomes the matrix of the overlap between the two basis.

Connection with GWT

$$\text{pf} \begin{bmatrix} V^T U & V^T \mathbf{p}^\dagger & V^T R^T \mathbf{q}'^T & V^T R^T V'^* \\ -\mathbf{p}^* V & \mathbf{q}^* \mathbf{p}^\dagger & \mathbf{q}^* R^T \mathbf{q}'^T & \mathbf{q}^* R^T V'^* \\ -\mathbf{q}' R V & -\mathbf{q}' R \mathbf{q}^\dagger & \mathbf{p}' \mathbf{q}'^T & \mathbf{p}' V'^* \\ -V'^\dagger R V & -V'^\dagger R \mathbf{q}^\dagger & -V'^\dagger \mathbf{p}'^T & U'^\dagger V'^* \end{bmatrix}.$$

equals (up to a phase) to

$$\text{pf} \begin{bmatrix} V^T U & V^T R^T V'^* & V^T \mathbf{p}^\dagger & V^T R^T \mathbf{q}'^T \\ -V'^\dagger R V & U'^\dagger V'^* & -V'^\dagger R \mathbf{q}^\dagger & -V'^\dagger \mathbf{p}'^T \\ -\mathbf{p}^* V & \mathbf{q}^* R^T V'^* & \mathbf{q}^* \mathbf{p}^\dagger & \mathbf{q}^* R^T \mathbf{q}'^T \\ -\mathbf{q}' R V & \mathbf{p}' V'^* & -\mathbf{q}' R \mathbf{q}^\dagger & \mathbf{p}' \mathbf{q}'^T \end{bmatrix}.$$

Aitken's formula: If

$$A = \begin{pmatrix} T & Q \\ -Q^T & S \end{pmatrix} \quad \text{pf}(A) = \text{pf}(T) \text{pf}(S + Q^T T^{-1} Q)$$

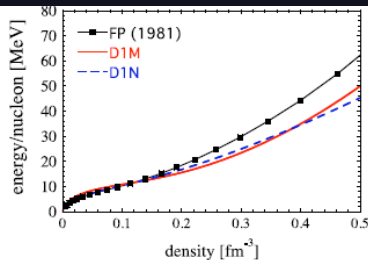
Note that $\text{pf}(T) \approx \langle \phi | \phi' \rangle$ and therefore the whole set of contractions is in $\text{pf}(S + Q^T T^{-1} Q)$. *Work in progress !*

Johann Friedrich Pfaff (sometimes spelled Friederich; born Stuttgart, 22 December 1765, died Halle, 21 April 1825) was a German mathematician. He was described as one of Germany's most eminent mathematicians during the 19th century. He studied integral calculus, and is noted for his work on partial differential equations of the first order (Pfaffian systems as they are now called) which became part of the theory of differential forms; and as Carl Friedrich Gauss's formal research supervisor.



Skyrme, Gogny, RMF

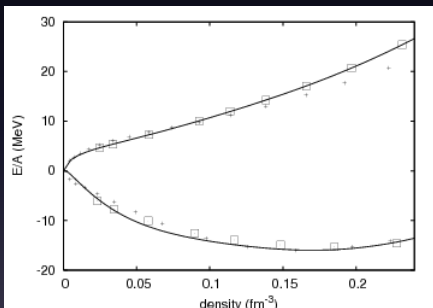
- Fixed central parts with ≈ 10 parameters
- Fitted to nuclear matter EoS obtained in realistic calculations (BHF + AV18, etc)



- Hard to reproduce the EoS in the whole range of relevant densities
- Proliferation of parametrizations

BCPM

- Fit the EoS with a given function of ρ and use the LDA for finite nuclei.



- Similar to DFT strategy to **guess** the unknown exchange terms
- Similar idea by Fayans in 2000

BCP EDF

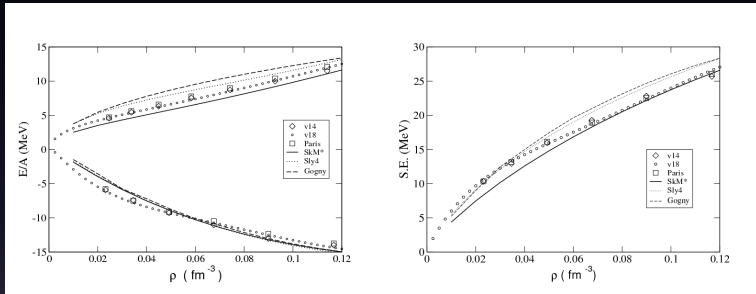
Polynomial fit to realistic EoS to produce a function of ρ .
Invoke LDA to obtain an EDF for finite nuclei (+ some cooking)

M.Baldo, P.Schuck and X. Viñas, Phys. Lett. B663 (2008) 390
Barcelona, Catania, Paris

Requirements

- Not demanding in terms of computer resources
- Integer powers of the density (beyond mean field)
- Mass table quality for binding energies and radii (for astrophysical applications !)
- Suited to accurately describe other properties like
 - Quadrupole and octupole deformation
 - Fission
 - Moments of inertia
- Good behavior "beyond mean field" (correlations are very important)

Realistic EoS



M. Baldo, C. Maieron, P. Schuck and X. Viñas, Nucl. Phys. **A736** (2004) 241

- Bethe-Brueckner + Converged hole line expansion
- AV18 + Three body forces (Carlson, Schiavilla, Pandharipande, Wiringa)
- Symmetric + Neutron EoS
- For other asymmetries a quadratic interpolation is used

$$e = e_n \beta^2 + e_s (1 - \beta^2)$$

$$\text{with } \beta = (\rho_n - \rho_p) / \rho$$

Fitting the EoS

The symmetric (s) and neutron (n) matter EoS are now fitted with polynomials P_s and P_n of the total density ρ

$$P_s(\rho) = \begin{cases} \sum_{k=1}^5 a_k^{(n)} x^k & x < 1 \\ P_s(\rho_0) + a_1(x-1) + a_2(x-1)^2 & x > 1 \end{cases}$$

$$P_n(\rho) = \sum_{k=1}^5 b_k^{(n)} x^k$$

with $x = \rho/\rho_0$ and $\rho_0 = 0.16\text{fm}^{-3}$

- Can be used up to $\rho = 0.5\text{ fm}^{-3}$ (0.24 in former fits)
- The interpolating polynomial for symmetric matter has been constrained to allow a minimum exactly at the energy $E/A = -16\text{MeV}$ and Fermi momentum $k_F = 1.36\text{fm}^{-1}$, i.e. $\rho_0 = 0.16\text{ fm}^{-3}$.
- Integer powers of the density (unlike expansions in k_F)

Fitting the EoS, results

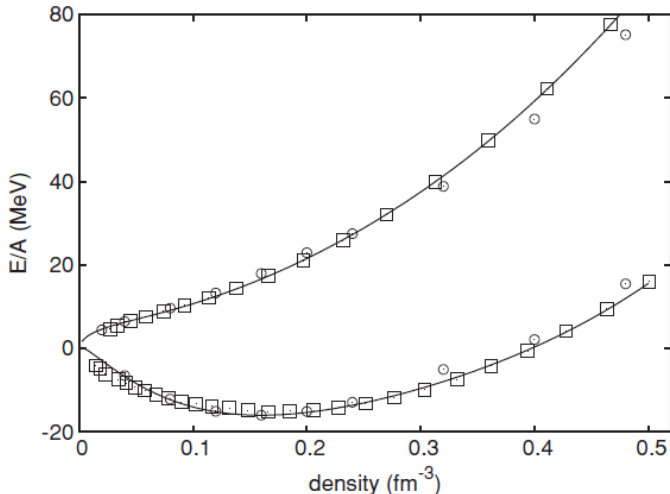


Figure 1. EOS of symmetric and neutron matter obtained by the microscopic calculation (squares) and the corresponding polynomial fits (solid lines). For comparison the microscopic EOS of [26] are also displayed by open circles.

The BCP functional

In the spirit of the LDA it is proposed to use the previous fit in finite nuclei just replacing the nuclear matter density ρ by the finite nuclei one $\rho(\vec{r})$.

The energy of a finite nucleus is given by

$$E = T_0 + E_{int}^{\infty} + E_{int}^{FR} + E^{s.o.} + E_C + E_{pair}.$$

where

$$E_{int}^{\infty}[\rho_p, \rho_n] = \int d\vec{r} [P_s(\rho)(1 - \beta^2) + P_n(\rho)\beta^2] \rho$$

with $\rho(\vec{r}) = \rho_n(\vec{r}) + \rho_p(\vec{r})$ and $\beta(\vec{r}) = (\rho_n(\vec{r}) - \rho_p(\vec{r}))/\rho(\vec{r})$

The other terms are the kinetic energy T_0 , a surface term E_{int}^{FR} , the spin-orbit energy $E^{s.o.}$, the Coulomb term E_C and finally the pairing energy E_{pair}

Remaining contributions to the EDF

- *Phenomenological surface contribution*

$$E_{int}^{FR}[\rho_n, \rho_p] = \frac{1}{2} \sum_{t,t'} \left\{ \iint d\vec{r} d\vec{r}' \rho_t(\vec{r}) v_{t,t'}(\vec{r} - \vec{r}') \rho_{t'}(\vec{r}') - \gamma_{t,t'} \int d\vec{r} \rho_t(\vec{r}) \rho_{t'}(\vec{r}) \right\}$$

with $v_{t,t'}(r) = V_{t,t'} e^{-r^2/r_0^2}$ and $\gamma_{t,t'} = \int d\vec{r} v_{t,t'}(r)$

$V_{n,n} = V_{p,p} = V_L$, $V_{n,p} = V_{p,n} = V_U$ and r_0 are free parameters to be fitted using finite nuclei data

- *Coulomb*

Direct $E_C^H = (1/2) \iint d\vec{r} d\vec{r}' \rho_p(\vec{r}) |\vec{r} - \vec{r}'|^{-1} \rho_p(\vec{r}')$

Exchange: $E_C^{ex} = -(3/4)(3/\pi)^{1/3} \int d\vec{r} \rho_p(\vec{r})^{4/3}$

- *Spin-Orbit*

$$\hat{v}_{ij}^{so} = iW_{LS}(\vec{\sigma}_i + \vec{\sigma}_j) \cdot [\vec{k}' \times \delta(\vec{r}_i - \vec{r}_j)\vec{k}]$$

Free parameters

V_U , V_L , W_{LS} and r_0

Remaining contributions to the EDF

- Pairing Correlations

Zero-range interaction, tailored to $m=m^*$,

$$v^{\rho\rho}(\rho(\vec{r})) = \frac{v_0}{2} \left[1 - \eta \left(\frac{\rho(\vec{r})}{\rho_0} \right)^\alpha \right], \quad \rho_0 = \frac{2}{3\pi^2} k_F^3.$$

L.N. Oliveira, E.K.U. Gross and W. Kohn, Phys. Rev. Lett. **60** (1988) 2430.

E. Garrido, P. Sarriguren, E. Moya de Guerra, and P. Schuck, Phys. Rev. C **60**, 064312 (1999)

Parameters fitted to reproduce Gogny's pairing gap in nuclear matter

- Two-body center of mass correction
Pocket formula based on HO

M.N. Butler, D.W.L. Sprung and J.Martorell, Nucl. Phys. **A422**, 157 (1984).

Fitting procedure (BCP1 and 2)

The free parameters, V_L , V_U , r_0 and W_{LS} are fitted to reproduce

- the binding energies of the spherical nuclei ^{16}O , ^{40}Ca , ^{48}Ca , ^{72}Ni , ^{90}Zr , ^{116}Sn , ^{124}Sn , ^{132}Sn , ^{204}Pb , ^{208}Pb , ^{214}Pb , and ^{210}Po
- the charge radii $r_c = \sqrt{r_p^2 + 0.64}$ fm of the spherical nuclei ^{16}O , ^{40}Ca , ^{48}Ca , ^{90}Zr , ^{116}Sn , ^{124}Sn , ^{204}Pb , ^{208}Pb and ^{214}Pb .

	r_0 (fm)	V_L (MeV)	V_U (MeV)	W_{LS} (MeV)
BCP 1	1.05	-93.520	-60.577	113.829
BCP 2	1.25	-33.700	-32.483	110.812

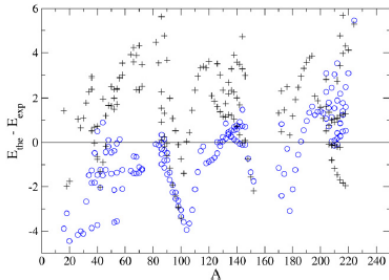


Fig. 2. Differences between the theoretical and experimental energies. Calculations are performed using the BCP1 functional (open circles) and the D1S parameter set (crosses) [45].

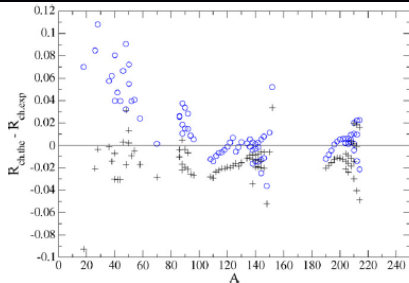


Fig. 3. Differences between the theoretical and experimental charge rms radii. Calculations are performed using the BCP1 energy functional (open circles) and D1S parameter set (crosses) [45].

Using 161 spherical nuclei

	BCP1	BCP2	D1S	NL3	SLy4	
rms_E	1.775	2.057	2.414	3.582	1.711	MeV
rms_R	0.031	0.028	0.020	0.020	0.024	fm

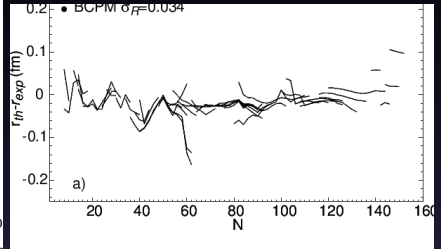
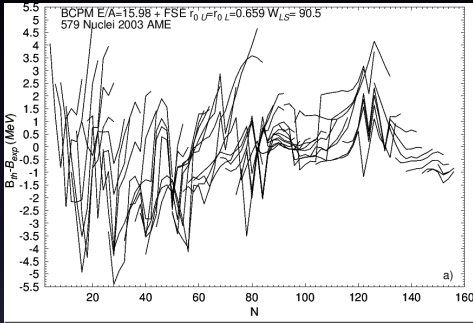
BCPM (just out of the oven)

In

$$E_{int}^{FR}[\rho_n, \rho_p] = \frac{1}{2} \sum_{t,t'} (\int \int d\vec{r} d\vec{r}' \rho_t(\vec{r}) v_{t,t'}(\vec{r}-\vec{r}') \rho_{t'}(\vec{r}') - \gamma_{t,t'} \int d\vec{r} \rho_t(\vec{r}) \rho_{t'}(\vec{r}))$$

- Set $\gamma_{t,t'}$ to zero and fix V_U and V_L to reproduce the quadratic terms of the polynomial fits of symmetric and neutron matter.
- To give some flexibility, introduce two ranges r_{0L} and r_{0U}
- Do global fits to all even-even nuclei by exploring the space of parameters
- E/A is also explored (vary fit parameters of EOS)
- New fit to NM EoS (avoiding some wiggles)
- W_{LS} is somehow fixed by magic numbers to be around 95
- It turns out that the fit favors $r_{0L} = r_{0U}$

BCPM



$$\sigma_E(559) = 1.58 \text{ MeV}$$

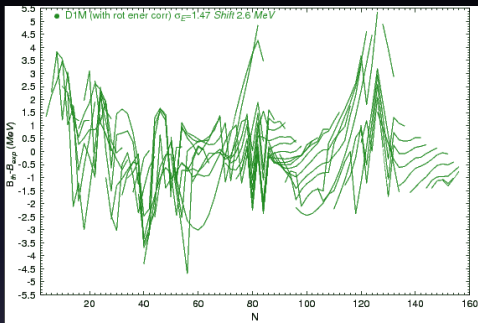
$$\sigma_{EA} > 40(536) = 1.51 \quad \sigma_{EA} > 80(452) = 1.35 \text{ MeV}$$

$$\sigma_R(315) = 0.031 \text{ fm}$$

σ_E very sensitive to r_0

With just 2 + 1/2 parameters

Other interactions



- $\sigma_E(559) = 1.47 \text{ MeV}$
- Calculations performed under the same conditions as BCPM (even-even nuclei, E_{ROT} , infinite basis extrapolation.)
- No quadrupole correlation energy

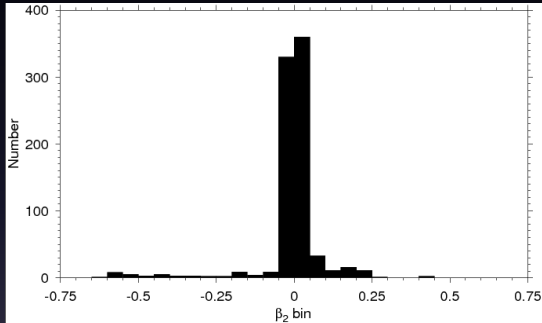
G. F. BERTSCH, B. SABBEY, AND M. UUSNÄKKI

TABLE II. Refits of various Skyrme parametrizations. The experimental data set is even-even nuclei of the 2003 mass table [10]. The last entry give the corresponding properties of the liquid drop model, Eq. (1), for comparison purposes. All energies are in mega-electron-volts.

Theory	r.m.s. residual	$a_s(c)$	$a_t(c)$
SLy4 [8]	1.7	-16.06	32.0
SkP-based [11]	1.7	-16.11	31.1
Bsk4-based [12]	1.7	-16.03	29.6
Skxce-based [13]	1.5	-16.10	31.0
LD	3.1	-15.6	23.3

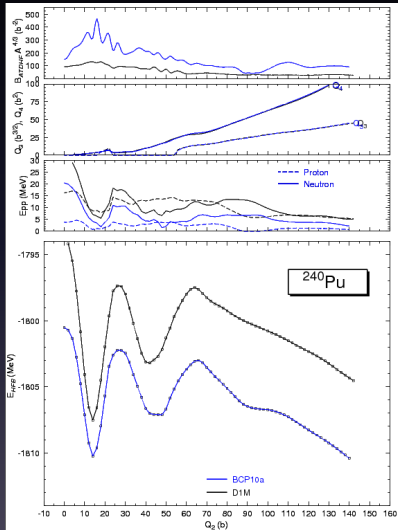
Popular Skyrme functionals

Global quadrupole deformation



Differences in GS β_2 deformation parameter according to BCPM and D1M Largest differences correspond to the region $A \approx 100$ of shape coexistence

Fission



- BCPM and D1M quite similar
- Lower barrier heights in BCP
- Larger collective masses
- Similar WKB half lives

- $\tau_{\text{BCPM}} = 2 \cdot 10^{29} \text{ s}$
- $\tau_{\text{D1M}} = 1.4 \cdot 10^{32} \text{ s}$
- $\tau_{\text{D1S}} = 1.5 \cdot 10^{26} \text{ s}$

Triaxiality not taken into account

BCP bibliography

- M. Baldo, P. Schuck and X. Viñas,
Phys. Lett. B663 (2008) 390
- L.M. Robledo, M. Baldo, P. Schuck y X. Viñas,
Phys. Rev C77, 051301 1-5 (R) (2008)
- L.M. Robledo, M. Baldo, P. Schuck y X. Viñas,
Phys. Rev C81, 034315 (1-13) (2010)
- X. Vinyes, L.M. Robledo, P. Schuck and M. Baldo,
Intl. J. of Mod. Phys. E18, 935 (2009)
- M. Baldo, L.M. Robledo, P. Schuck and X. Viñas,
Jour. of Phys. G37, 064015 (2010)