

odd- A nuclei and high- K isomeric states with the BCPM functional

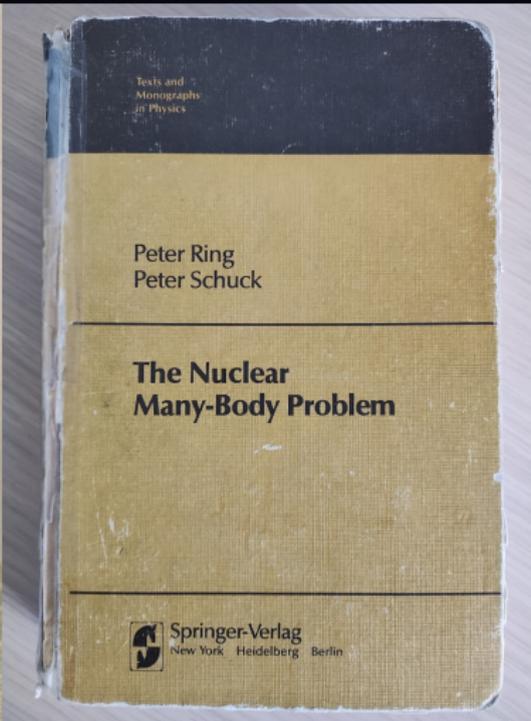
S.A. Giuliani and L.M. Robledo

Universidad Autónoma de Madrid, Madrid, Spain

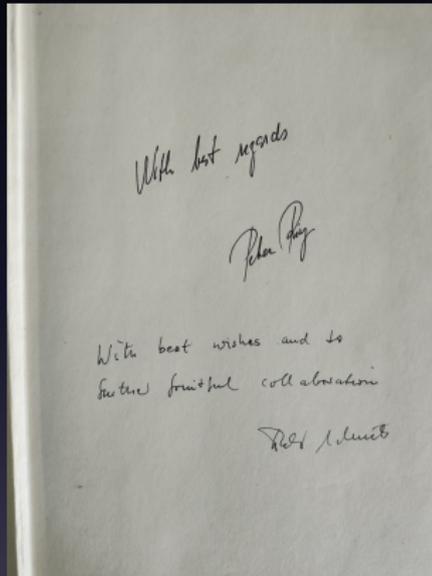
March 21st, 2023

A tribute to the memory of Peter Schuck, Orsay 2023

Peter Schuck



the connection



Madrid, January 2007

Peter and Xavier (and Jorge)



Paris, February 2011

BCP family of functionals

- BCP1 and BCP2 (2008)
Basic idea introduced
(fit to EOS with a polynomial in density)
PLB 636, 390 (2008)
- BCPM (2013)
Reduction in the number of parameters by some
assumptions in the surface term
PRC 87, 064305 (2013)
- BCPM* (2016)
Realistic effective mass
PRC 95, 014318 (2017)

Today we will focus on the extension of BCPM to the realm of odd-A nuclei

Effective interactions

Bare nucleon-nucleon

Bare nucleon-nucleon interaction is well known at long distances. At short distances the repulsive core is less known. Three body forces are more or less understood.

Short range in-medium correlations

Short range in-medium correlations (Pauli blocking) "cancel out" the repulsive core and yield a smooth effective in medium interaction

Effective interactions

Handling of short range correlations requires Brueckner-like methods which are extremely hard to implement in finite nuclei. The smooth effective in-medium interaction is replaced by phenomenological effective interactions like Skyrme, Gogny or RFM

Skyrme/Gogny/RMF

Non-relativistic Skyrme /Gogny

Central part, spin-orbit, Coulomb and a phenomenological density dependent term (usually involving non-integer powers of the density)

- Skyrme: Zero range central part $\delta(\vec{r} - \vec{r}') +$ gradient terms
- Gogny: Finite range central part $\exp(-(\vec{r} - \vec{r}')^2/\mu^2)$

RMF uses a relativistic lagrangian with external mesonic fields (densities)

10-15 params fitted to nuclear matter ($E/A, k_F, K, \dots$) and finite nuclei (mostly spherical at the valley of stability).

\approx 300 Skyrme parametrizations, 3 Gogny, and \approx 15 RMF

- Most are tailored to specific phenomena
- Divergent results when there is no experimental data

Recent strategies

Nuclear matter input

Use more information from symmetric and neutron matter EoSs to constrain the parameters

- $\rho < \rho_0$ relevant at the surface of finite nuclei
- Better neutron matter EoS should improve description of neutron rich nuclei

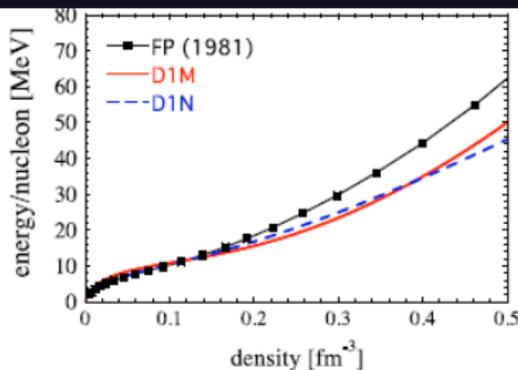
Skyrme SLy, SV, UNDEFX, HFB-21, Gogny D1N and D1M, etc

Global fit to finite nuclei

- Use binding energies of all finite nuclei as input to the fit.
- Deformed nuclei are relevant

Skyrme, Gogny, RMF

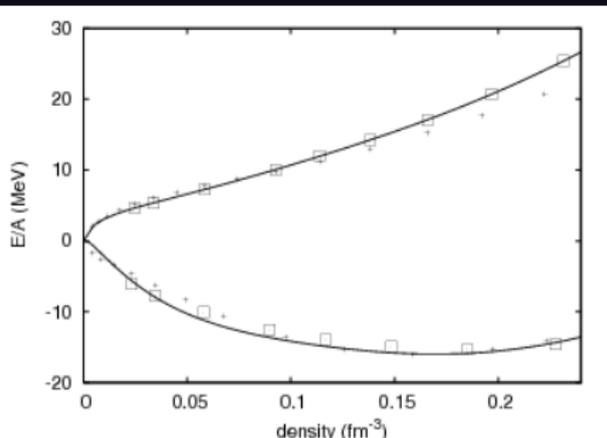
- Fixed central parts with ≈ 10 parameters
- Fitted to realistic nuclear matter EoS (BHF + AV18, etc)



- Not so easy to reproduce the EoS in the whole range of relevant densities
- Proliferation of parametrizations

The idea

- Starting from a polynomial fit to a microscopic EoS, both for symmetric and neutron matter, use the LDA for finite nuclei.



- Similar to DFT strategy to guess the unknown exchange terms
- Previous attempts by Fayans (2001) and Steiner (2005)

BCPM EDF

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

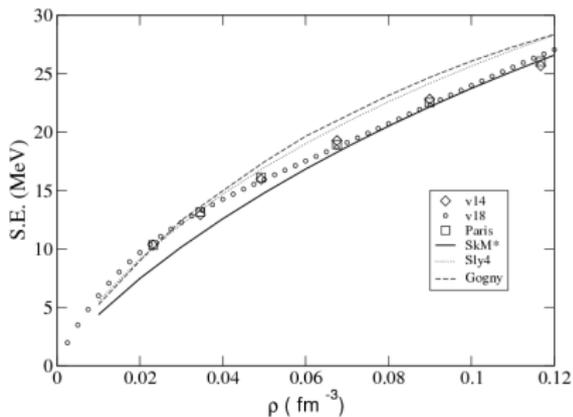
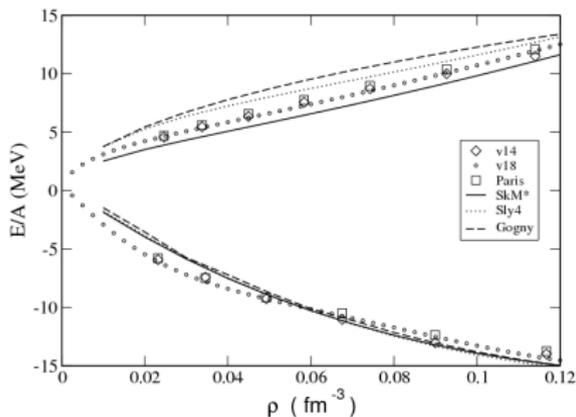
M.Baldo et al, *Phys. Rev. C*87 064305 (2013)

Barcelona, Catania, Paris, Madrid

Properties

- Integer powers of the density (good for beyond mean field)
- Mass table quality for binding energies and radii (good for astrophysical applications !)
- Reasonable description of
 - Quadrupole and octupole deformation
 - Fission / moments of inertia
 - Giant resonances
 - Crust of neutron stars in TF approach

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 fitted with polynomials P_s and P_n of the total density ρ

$$P_s(\rho) = \sum_{k=1}^5 a_k^{(n)} (\rho/\rho_0)^k$$

$$P_n(\rho) = \sum_{k=1}^5 b_k^{(n)} (\rho/\rho_{0n})^k$$

with $\rho_0 = 0.16 \text{ fm}^{-3}$ and $\rho_{0n} = 0.155 \text{ fm}^{-3}$

- Can be used up to $\rho = 0.625 \text{ fm}^{-3}$
- The interpolating polynomial for symmetric matter has been constrained to have a minimum around 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

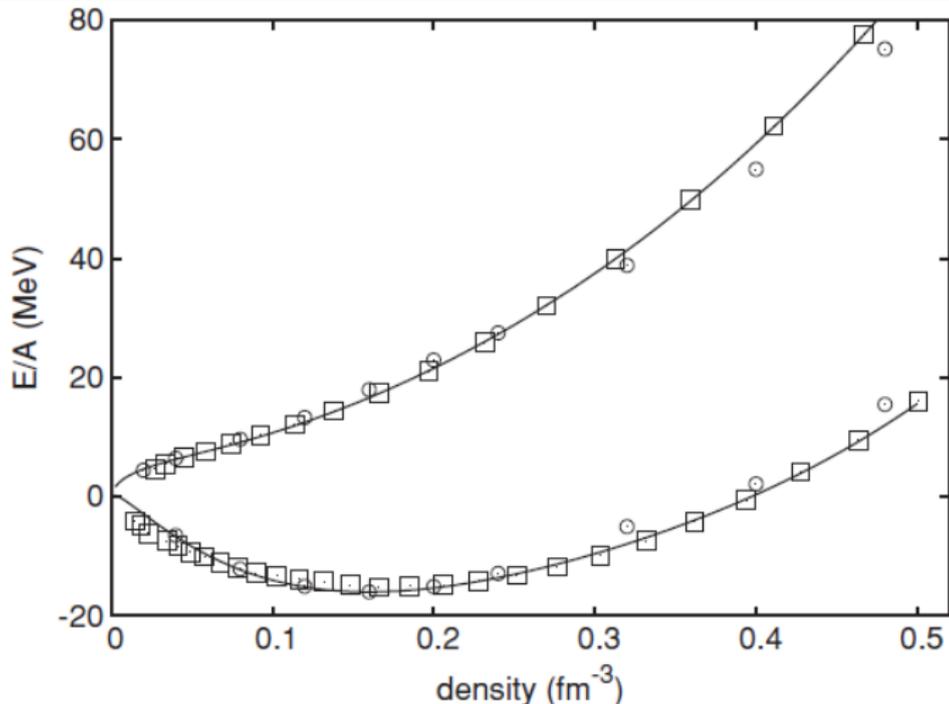


Figure 1. EOS of symmetric and neutron matter obtained by the microscopic calculation (squares) and the corresponding polynomial fits (solid lines). For comparison the microscopic EOS of [26] are also displayed by open circles.

The BCPM functional

In the spirit of the LDA, we use the previous polynomial fit on the density also in finite nuclei just replacing the nuclear matter density ρ by the its finite nuclei counterpart $\rho(\vec{r})$.

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*

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

with $v_{t,t'}(r) = V_{t,t'} e^{-r^2/r_0 t^2}$

$$V_{n,n} = V_{p,p} = V_L = \frac{2\tilde{b}_1}{\pi^{3/2} r_{0L}^3 \rho_0} \quad V_{n,p} = V_{p,n} = V_U = \frac{4a_1 - 2\tilde{b}_1}{\pi^{3/2} r_{0U}^3 \rho_0}$$

r_{0L} and r_{0U} 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: $E_C^{\text{ex}} = -(3/4)(3/\pi)^{1/3} \int d\vec{r} \rho_p(\vec{r})^{4/3}$

- *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

W_{LS} and r_{0L}, r_{0U}

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 protocol

it is better to fit deformed nuclei as they are more numerous and more "mean field" like (additional correlations are mostly static, not dynamic as in spherical nuclei ...)

We take 579 even-even nuclei (spherical and deformed) with known experimental binding energies (AMES2003)

The binding energy is the HFB mean field energy supplemented with the rotational energy correction and an estimation of the effect of the finite size of the basis.

From a preliminary fit with spherical nuclei one concludes that $r_{0L} = r_{0U}$ is a good choice

Spin orbit strength fixed to reasonable values ($W_{LS} \approx 90 = 0.7 \times 130$)

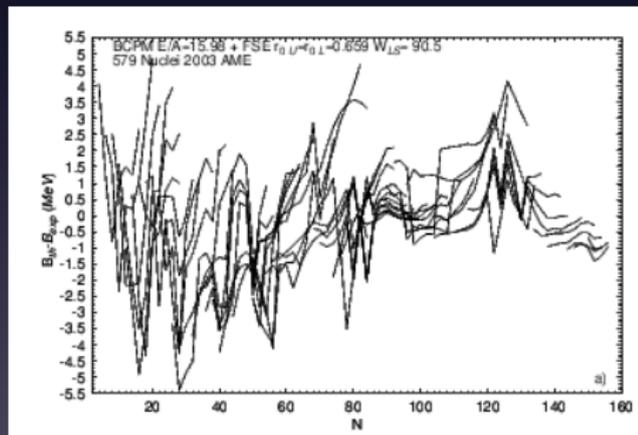
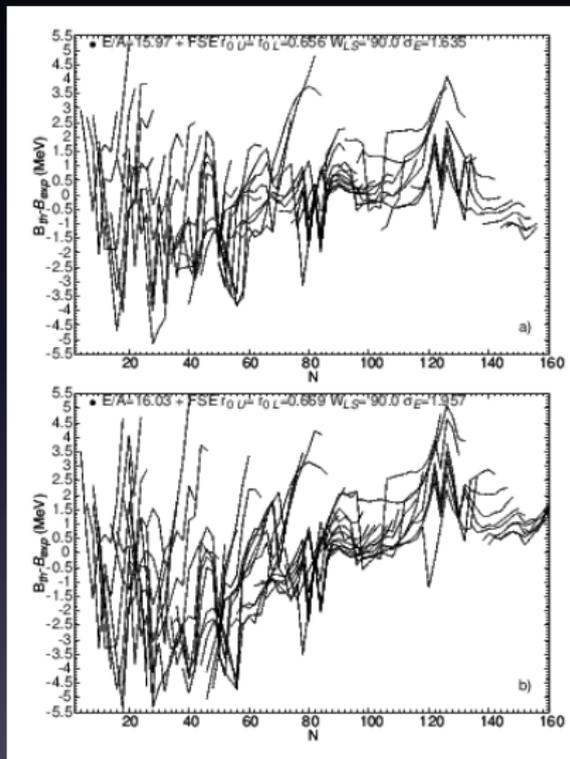
Pairing strength also fixed

E/A

Slope of ΔB depends on E/A at the minimum of the polynomial fit of the EoS

E/A is a new parameter (Volume energy)

$r_{0L} = r_{0U}$ drives the surface energy



BCPM

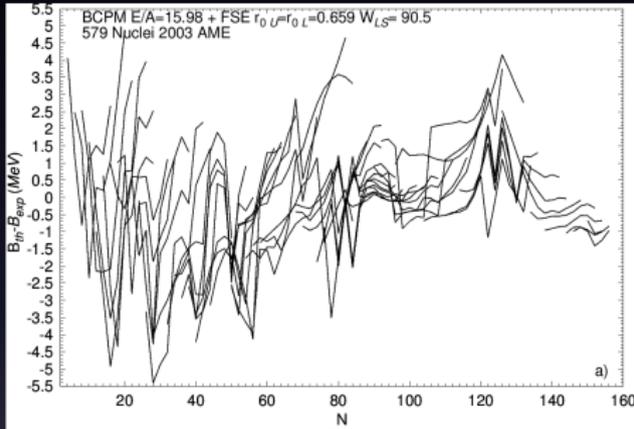
BCPM

- $E/A = 15.98$ MeV
- $r_{0L} = r_{0U} = 0.659$ fm
- $W_{LS} = 90.5$ MeV fm⁻³

Nuclear matter properties

B/A	ρ_0	m/m^*	J	L	K_0	K'	K_{sym}
-15.98	0.16	1.00	31.90	52.96	212.4	879.6	-96.75

BCPM binding energies



$$\sigma_E(579) = 1.58 \text{ MeV}$$

$$\sigma_{EA} > 40(536) = 1.51,$$

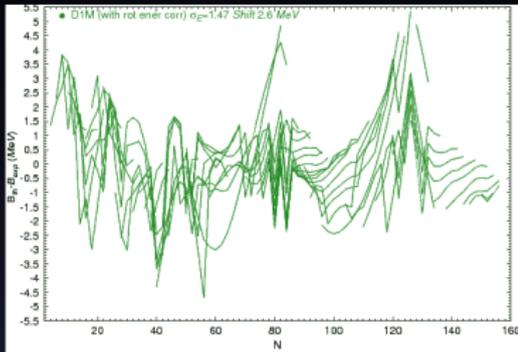
$$\sigma_{EA} > 60(496) = 1.45$$

$$\sigma_{EA} > 80(452) = 1.35 \text{ MeV}$$

$$\sigma_R(313) = 0.027 \text{ fm}$$

- $\sigma_E = \text{sqrt}(\sum (B_{th} - B_{exp})^2 / N)$
- Better for heavier nuclei
- $r^2 = r_{point}^2 + 0.875^2$

A comparison with Gogny

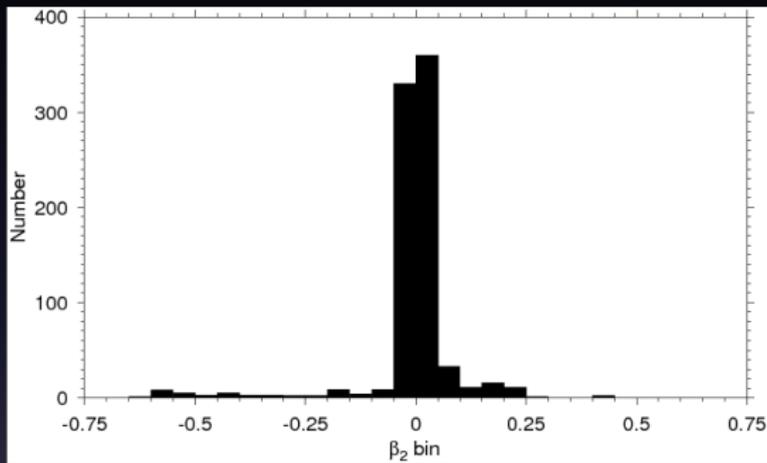


D1M

- $\sigma_E(579) = 1.47 \text{ MeV}$
- Calculations performed under the same conditions as BCPM (even-even nuclei, E_{ROT} , infinite basis extrap.)
- There is no quadrupole zero point energy

$\sigma(E)$	D1S	D1M	D1N
HFB	3.48	5.08	4.88
HFB+ E_{ROT}	2.15	2.96	2.84
HFB + Shift	2.53 (2.4)	2.02 (4.7)	2.02 (4.5)
HFB+ E_{ROT} +Shift	2.14 (0.2)	1.47 (2.6)	1.45 (2.4)

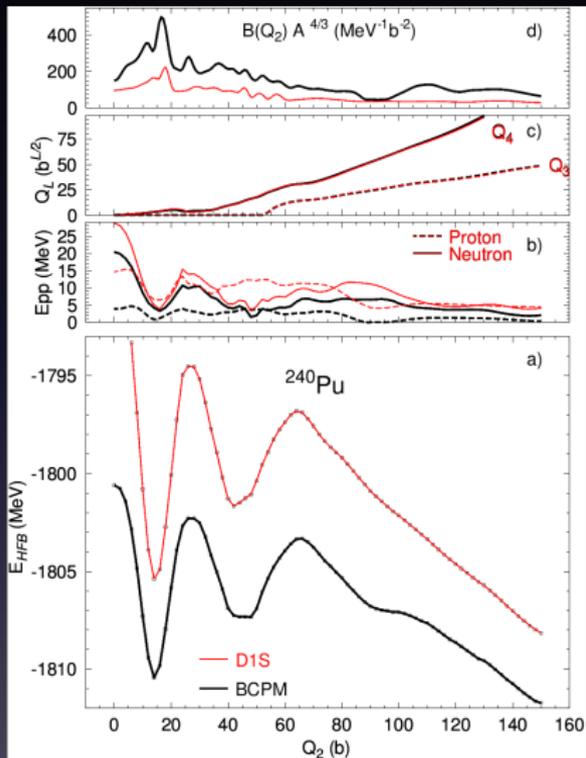
Global quadrupole deformation



Histogram where bin i reckons number of nuclei with $0.025(i - 1) < \beta_2(D1S) - \beta_2(BCPM) < 0.025i$

Largest differences correspond to the region $A \approx 100$ of shape coexistence

Fission BCPM

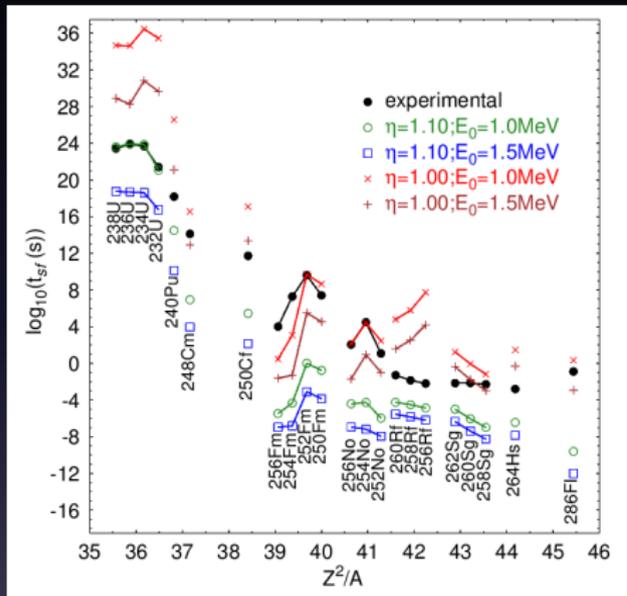


- BCPM and D1S are similar
- Lower barrier heights in BCPM
- Larger collective masses
- Similar WKB half lives

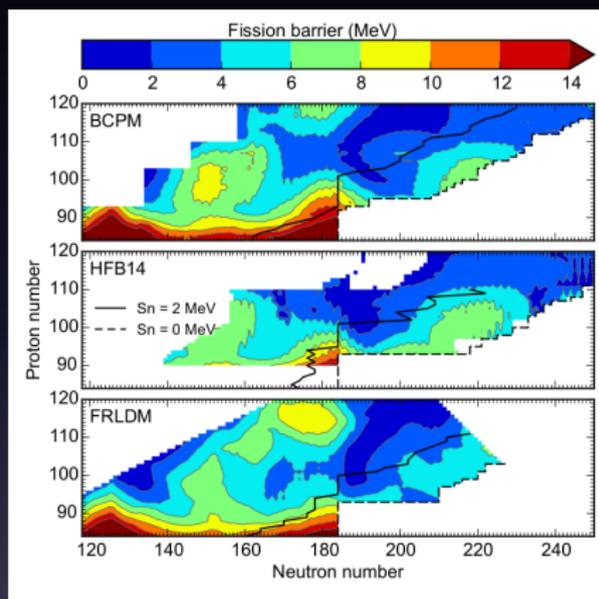
- $\tau_{\text{BCPM}} = 2 \cdot 10^{29} \text{ s}$
- $\tau_{\text{D1M}} = 1.4 \cdot 10^{32} \text{ s}$
- $\tau_{\text{D1S}} = 1.5 \cdot 10^{26} \text{ s}$

No triaxiality taken into account at the first barrier

Fission BCPM



Physical Review C 88 054325
(2013)

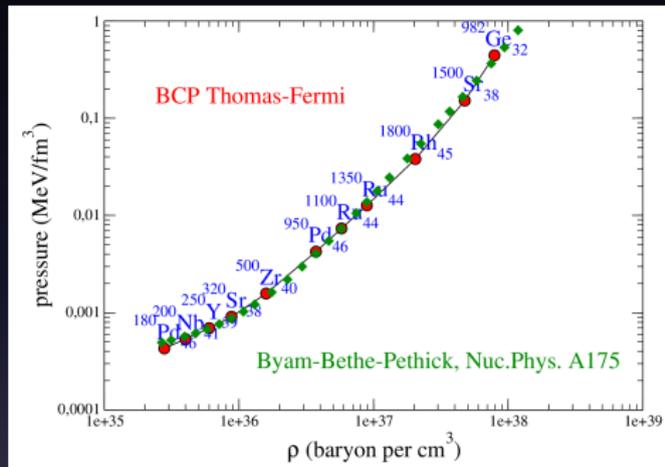
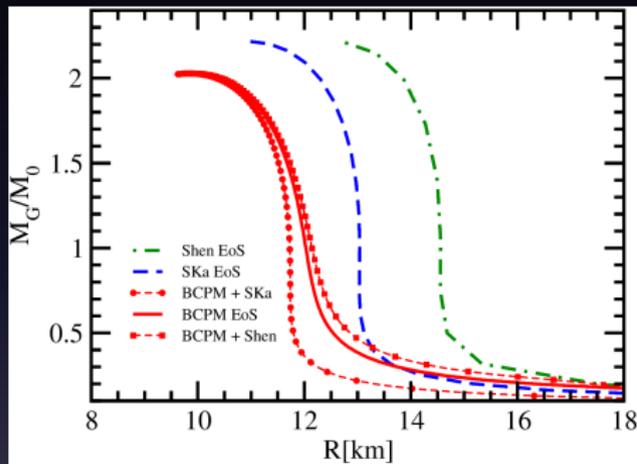


arxiv: with S. Giuliani and G.
Martinez-Pinedo

Isoscalar Monopole Giant Resonances

Nucleus	$E_3(M)$	$E_1(M)$	$E_3(Q)$	Exp(M)	Exp(Q)
^{90}Zr	19.06	18.32	13.34	17.81 ± 0.32	14.30 ± 0.40
^{144}Sm	16.44	15.62	11.45	15.40 ± 0.30	12.78 ± 0.30
^{208}Pb	14.49	13.84	10.16	13.96 ± 0.20	10.89 ± 0.30
^{112}Sn	17.75	16.83	12.36	16.1 ± 0.1	13.4 ± 0.1
^{114}Sn	17.64	16.75	12.28	15.9 ± 0.1	13.2 ± 0.1
^{116}Sn	17.53	16.66	12.21	15.8 ± 0.1	13.1 ± 0.1
^{118}Sn	17.41	16.55	12.15	15.6 ± 0.1	13.1 ± 0.1
^{120}Sn	17.29	16.43	12.09	15.4 ± 0.2	12.9 ± 0.1
^{122}Sn	17.18	16.32	12.04	15.0 ± 0.2	12.8 ± 0.1
^{124}Sn	17.06	16.21	12.44	14.8 ± 0.2	12.6 ± 0.1
^{106}Cd	18.09	17.07	12.70	16.50 ± 0.19	
^{110}Cd	17.85	16.97	12.49	16.09 ± 0.15	13.13 ± 0.66
^{112}Cd	17.74	16.83	12.38	15.72 ± 0.10	
^{114}Cd	17.59	16.73	12.29	15.59 ± 0.20	
^{116}Cd	17.44	16.52	12.19	15.40 ± 0.12	12.50 ± 0.66

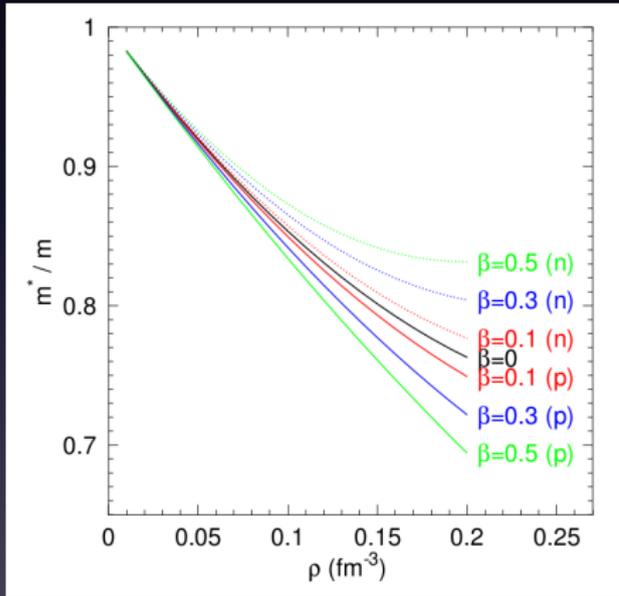
Neutron Stars



Two solar masses !
Reasonable results for pressure !

BCPM*

The effective mass of BCPM is one, a property that causes some trouble in describing the excitation energy of collective excitations (GQR)



Realistic effective mass m^*

In order to introduce an effective mass we replace

$$\frac{\hbar^2}{2m} \tau \rightarrow \frac{\hbar^2}{2m^*} \tau - B(\rho) \tau^\infty$$

with

$$B(\rho) = \frac{\hbar^2}{2m} \left(\frac{m}{m^*} - 1 \right)$$

There are no issues with Galilean invariance because we are dealing with even-even nuclei

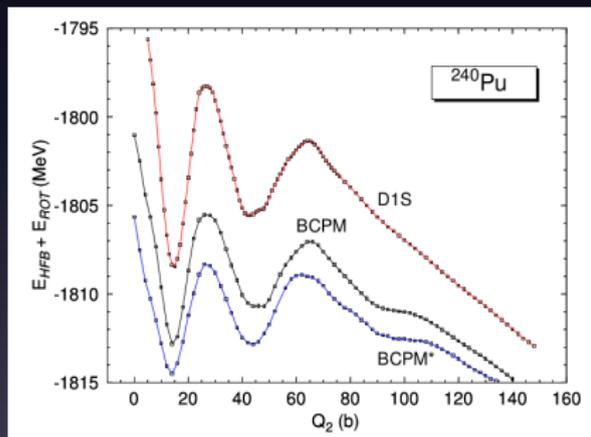
Simple polynomial fit of m^*

Phys. Rev C 95, 014318 (2017)

BCPM*

	W_{LS} (MeV fm ⁵)	r_{0U} (fm)	r_{0L} (fm)	E/A (MeV)	σ_E (MeV)	σ_R (fm)
BCPM	90.5	0.659	0.659	15.98	1.61	0.027
BCPM*	112	0.7520	0.7520	15.98	1.65	0.024

New fit with
AME2012

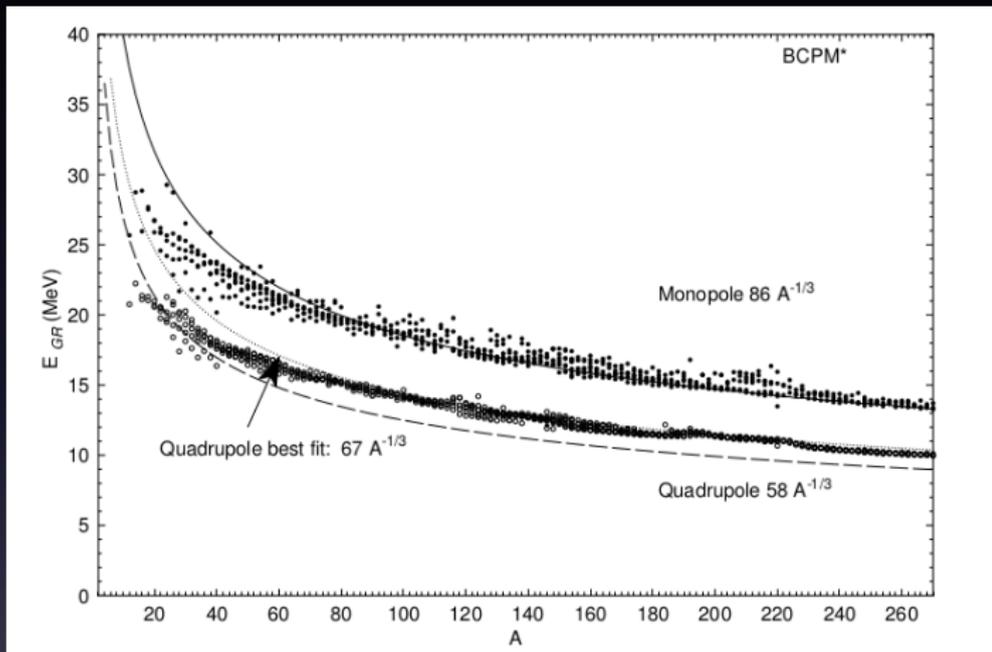


Fission path almost unaltered

	BCPM*			BCPM			Exp		
	E_A	E_B	E_I	E_A	E_B	E_I	E_A	E_B	E_I
²³⁴ U	5	5.8	1.8	5.6	5.6	2.	4.8	5.5	-
²⁴⁰ Pu	6.2	5.5	1.7	7.3	5.8	2.1	6	5.15	2.8
²⁴⁴ Pu	6.1	6.2	1.7	7.8	6.4	2.5	5.70	4.85	-
²⁴² Cm	6.3	4.3	1.1	7.4	4.5	1.5	6.65	5.0	1.9
²⁴⁶ Cm	6.5	4.7	1.1	8	5.5	2.1	6	4.8	-

Better fission barrier heights but
lower fission isomer excitation
energy

BCPM*



Better reproduction of the GQR energies (scaling approximation) than with BCPM

A lot of work remains to be done in order to assess the quality of BCPM*

what is next

- Other collective excitations (GDR, etc)
- Include triaxiality and high spin physics
- Odd-A nuclei. Need to define new time-odd terms
- Thermal effects
- Explore beyond mean field approaches like symmetry restorations
- Explore other pairing functionals
- ...

Odd-A and MQP excitations

- Time odd terms in the functional require polarized nuclear matter calculations
- Those are not available and therefore BCPM cannot be used to describe time-odd physics including
 - High spin physics
 - odd-A and odd-odd nuclei
 - Multi-quasiparticle excitations
- Odd-A and odd-odd nuclei can be treated with the Equal Filling Approximation (EFA)
- This approximation is equivalent to neglecting time-odd fields in the standard full blocking approach (FBA)
- It was shown with Skyrme forces that EFA and FBA provide quite similar results (see below)

Does it make sense to use the densities and pairing tensor of the EFA along with BCPM to analyze odd-A, odd-odd and MQP excitations ?

EFA

odd-A are described at the HFB level with a blocked wave function $\beta_{\mu_B}^+|\phi\rangle$

Everything depends upon the density and pairing tensors

$$\rho_{kk'}^{(\mu_B)} = \langle\phi|\beta_{\mu_B}\mathbf{c}_{k'}^+\mathbf{c}_k\beta_{\mu_B}^+|\phi\rangle \quad (1)$$

$$= \left(V^*V^T\right)_{kk'} + \left(U_{k'\mu_B}^*U_{k\mu_B} - V_{k'\mu_B}V_{k\mu_B}^*\right) \quad (2)$$

and

$$\kappa_{kk'}^{(\mu_B)} = \langle\phi|\beta_{\mu_B}\mathbf{c}_{k'}\mathbf{c}_k\beta_{\mu_B}^+|\phi\rangle \quad (3)$$

$$= \left(V^*U^T\right)_{kk'} + \left(U_{k\mu_B}V_{k'\mu_B}^* - U_{k'\mu_B}V_{k\mu_B}^*\right) \quad (4)$$

The terms depending upon μ_B break time reversal invariance

EFA

In the EFA, the time-reversal-breaking term is "averaged" in the density

$$\begin{aligned} \rho_{kk'}^{EFA} &= \left(V^* V^T \right)_{kk'} \\ &+ \frac{1}{2} \left(U_{k'\mu_B} U_{k\mu_B}^* - V_{k'\mu_B}^* V_{k\mu_B} + U_{k'\bar{\mu}_B} U_{k\bar{\mu}_B}^* - V_{k'\bar{\mu}_B}^* V_{k\bar{\mu}_B} \right) \end{aligned} \quad (5)$$
$$(6)$$

and pairing tensor

$$\begin{aligned} \kappa_{kk'}^{EFA} &= \left(V^* U^T \right)_{kk'} \\ &+ \frac{1}{2} \left(U_{k\mu_B} V_{k'\mu_B}^* - U_{k'\mu_B} V_{k\mu_B}^* + U_{k\bar{\mu}_B} V_{k'\bar{\mu}_B}^* - U_{k'\bar{\mu}_B} V_{k\bar{\mu}_B}^* \right) \end{aligned} \quad (7)$$
$$(8)$$

Every mean value is written replacing the "blocked" density and pairing tensor by the EFA ones.

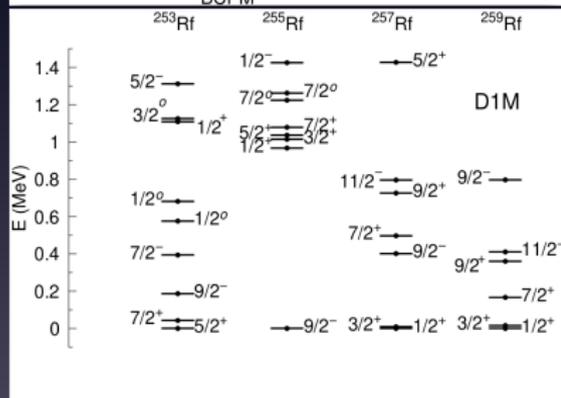
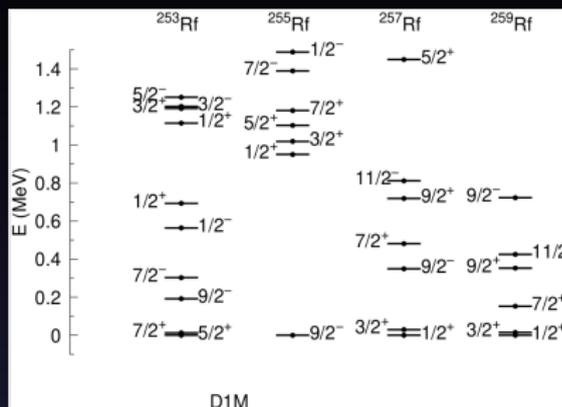
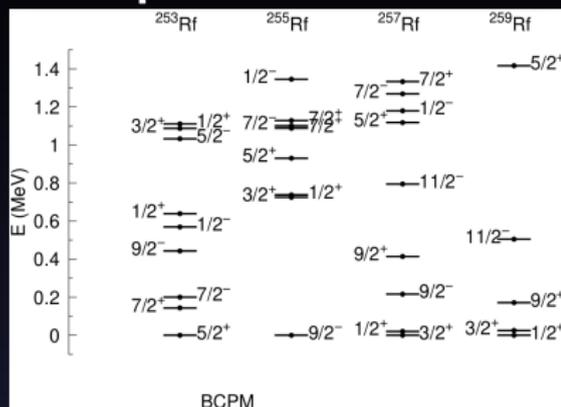
EFA

- The EFA can be viewed as a quantum statistical system where both $\beta_{\mu_B}^+ |\phi\rangle$ and $\beta_{\mu_B}^- |\phi\rangle$ are present with equal probability $1/2$.
- Introduce a quantum density operator \mathcal{D} ($\hat{\mathcal{D}}\beta_{\mu}^{\dagger} = \rho_{\mu}\beta_{\mu}^{\dagger}\hat{\mathcal{D}}$) and mean values are replaced by traces over multi-quasiparticle excitations
- Thanks to Gaudin's theorem (Wick's theorem for statistical averages) every mean value takes the standard form in terms of density and pairing tensor, but as a function of the statistical density and pairing tensor.
- The statistical density and pairing tensor are nothing but the EFA quantities
- The formalism of finite temperature can be borrowed
- As a consequence, EFA is a variational theory and gradient methods can be used to derive and solve the EFA-HFB equation.

Procedure

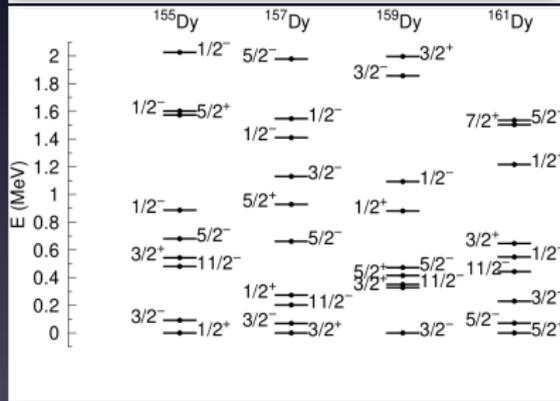
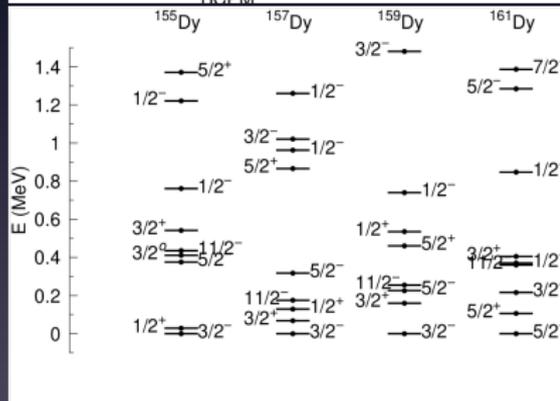
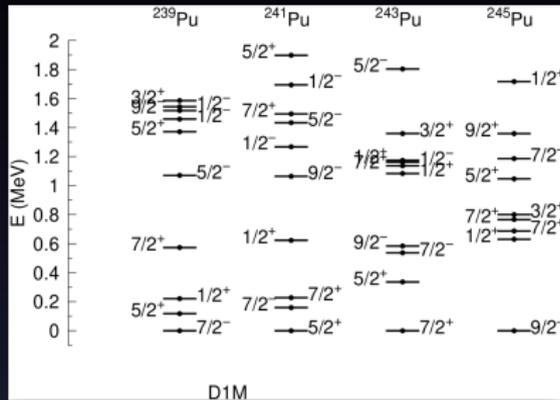
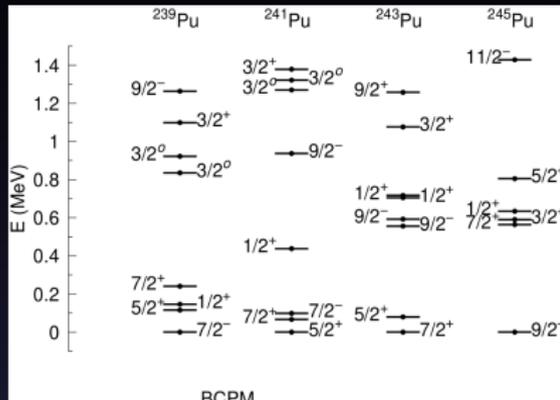
- Compute a fully paired HFB state $|\phi\rangle$ but constraining Z or N mean values to their odd target value
- Extract the 10-15 lowest quasiparticle state
- Selfconsistently solve the EFA-HFB equation
- It turns out that if there are no selfconsistent symmetries, the 10-15 EFA initial configurations will converge to the ground state
- To overcome this problem one could use orthogonality constraints, but we find easier to keep some symmetries like the K quantum number
- EFA states are labeled by K and we assume the equivalence between K and J
- Parity is allowed to break, but it is often preserved.
- If there are two or more quasiparticles with the same K and π they will likely converge to the lowest state (except if they have quite different deformations)

Examples

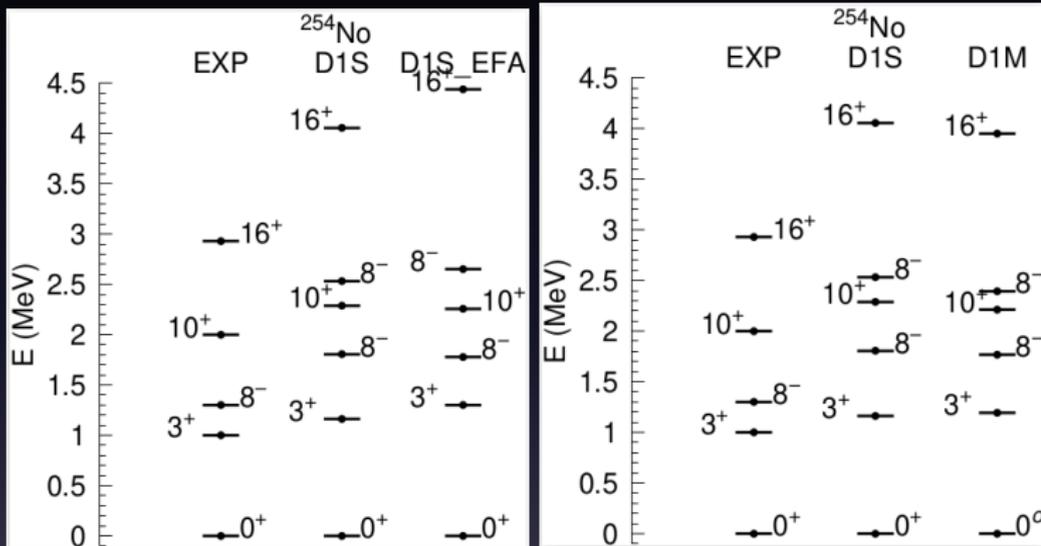


A comparison BCPM, D1M and D1M (full blocking)

Examples



Examples: EFA in High-K in ^{254}No



EFA also works for high-K isomeric states.

Work in progress suggests that BCPM predictions are also good in this case