The Barcelona-Catania-Paris-Madrid energy density functional

M. Baldo[a], L.M. Robledo[b], P. Schuck[c], X. Vinyes[d]

[a]Instituto Nazionale di Fisica Nucleare, Sezione di Catania, Catania, Italy
[b]Universidad Autónoma de Madrid, Madrid, Spain
[c]Institut de Physique Nucléaire, Orsay, France
[d]Universitat de Barcelona, Barcelona, Spain

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Nuclear Structure and Astrophysical Applications

ECT* European Centre for Theoretical Studies in Nuclear Physics and Related Areas

Effective interactions

Bare nucleon-nucleon

Bare nucleon-nucleon interaction 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 (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, ...) 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 EoS 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

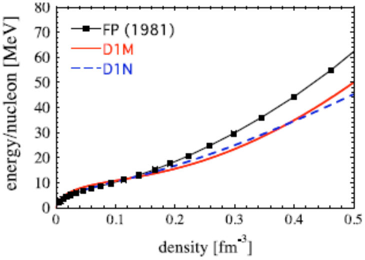
Skyrme SLy, SV, UNDEFX, HFB-21, Gogny D1N and D1M, etc

Global fit to finite nuclei

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

Skyrme, Gogny, RMF

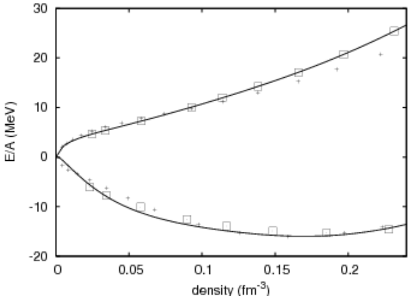
- Fixed central parts with ≈ 10 parameters
- Fitted to realistic nuclear matter EoS (BHF + AV18, etc)



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

the idea

- Starting from a microscopic EoS 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)

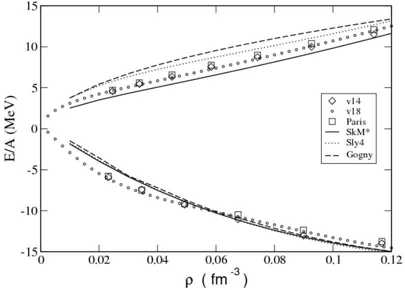
M.Baldo et al, Phys. Rev. C87 064305 (2013)

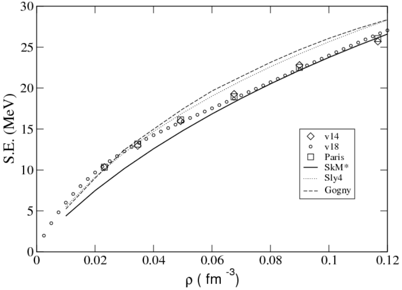
Barcelona, Catania, Paris, Madrid

Requirements

- Integer powers of the density (beyond mean field)
- Mass table quality for binding energies and radii (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

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

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

- Can be used up to $\rho = 0.625$ fm^{-3}
- The interpolating polynomial for symmetric matter has been constrained to have a minimum around the energy $E/A = -16MeV$ and Fermi momentum $k_F = 1.36fm^{-1}$, i.e. $\rho_0 = 0.16$ fm^{-3}.
- Integer powers of the density (unlike expansions in k_F)

Fitting the EoS, results

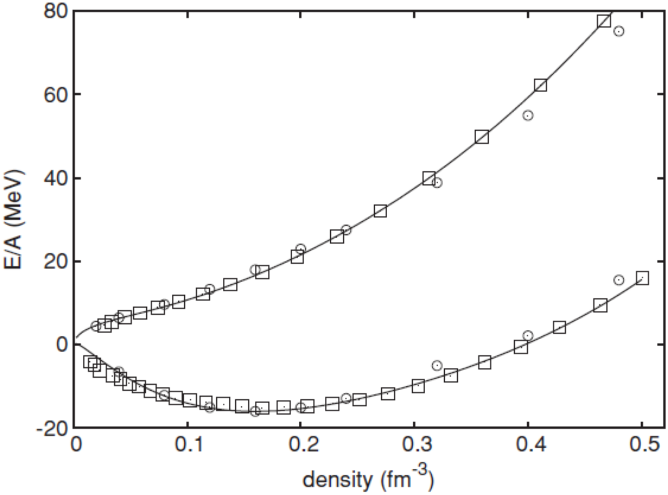


Figure 1. EOS of symmetric and neutron matter obtained by the microscopic calculation (squares) and the corresponding polynomial fits (solid lines). For comparison the microscopic EOS of [26] are also displayed by open circles.

The BCPM functional

In the spirit of the LDA 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

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

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}

M.Baldo et al. Phys. Lett. B663 (2008) 390; Phys. Rev. C87 064305 (2013)

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 $v_{t,t'}(r) = V_{t,t'}e^{-r^2/r_{0\,tt}{}^2}$

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

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

- *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*,

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

  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)

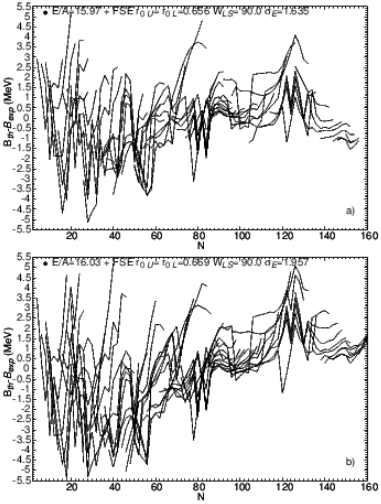
The binding energy is the HFB mean field energy supplemented with the rotational energy correction and an estimation of the effect of the finite size of the basis.

From a preliminary spherical fit we conclude 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

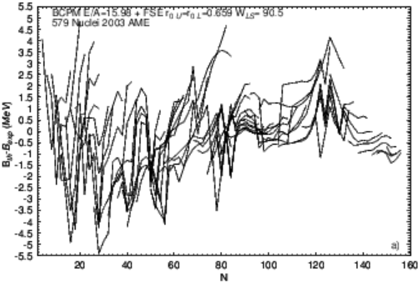
E/A



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



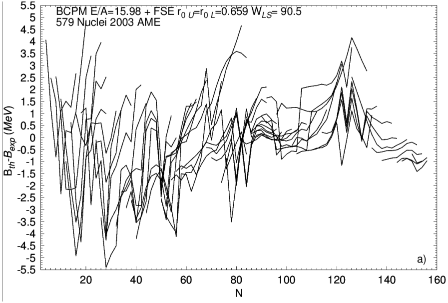
BCPM

- 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



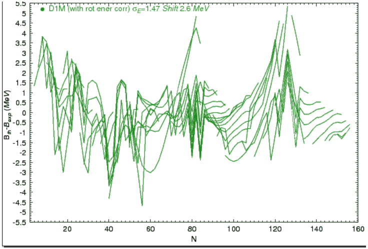
$\sigma_E(579) = 1.58$ MeV

$\sigma_E A > 40(536) = 1.51,$
$\sigma_E A > 60(496) = 1.45$
$\sigma_E A > 80(452) = 1.35$ MeV

$\sigma_R(313) = 0.027$ fm

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

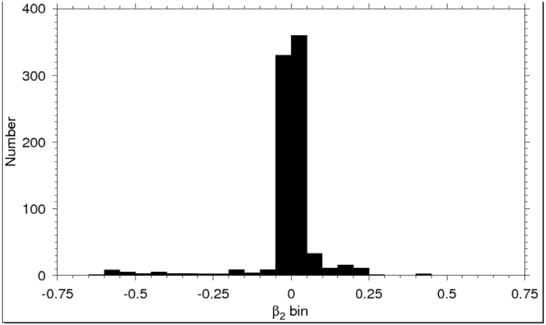
Gogny



- $\sigma_E(579) = 1.47$ 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)

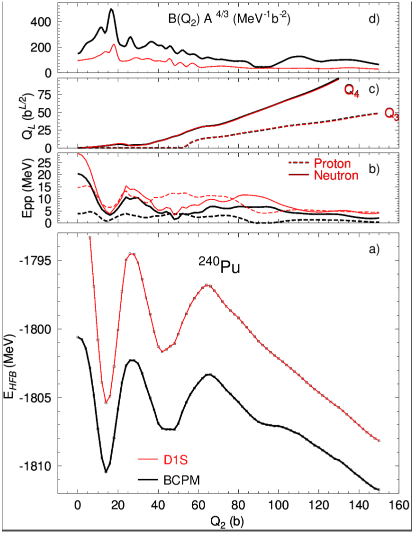
Global quadrupole deformation



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

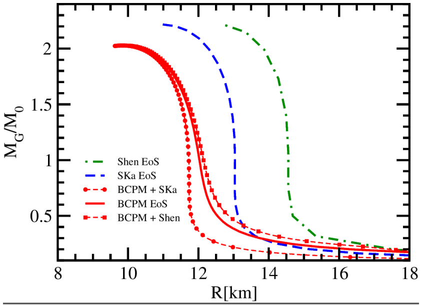
- $\tau_{\mathrm{BCPM}} = 2\,10^{29}$ s
- $\tau_{\mathrm{D1M}} = 1.4\,10^{32}$ s
- $\tau_{\mathrm{D1S}} = 1.5\,10^{26}$ s

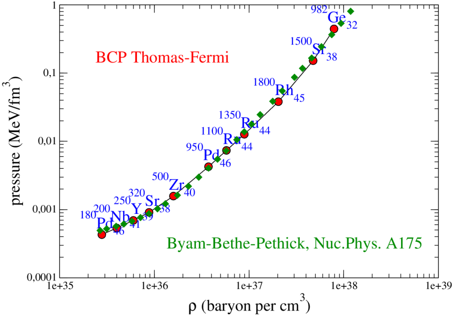
No triaxiality taken into account

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





what is next ....

- Effective mass
- Other collective excitations (GDR, etc)
- Include triaxiality and high spin physics
- Odd-A nuclei (in progress with spherical nuclei)
- Thermal effects
- Explore beyond mean field approaches like symmetry restorations
- Explore other pairing functionals
- ...

Conclusions

- A new EDF based on a fit to realistic EoS and the LDA is postulated
- It contains essentially two free parameters (apart from the ones of the nuclear matter fits)
- Its local character makes it fast on the computer
- Nice results for finite nuclei comparable to those of the performant Gogny forces
- Good binding energies and radii
- Fission and multipole deformation properties similar to D1S
- Reasonable description of the IMGR

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