Neutron Stars from the Kohn-Sham functional

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Plan of the talk

Introduction to the nuclear Kohn-Sham functional.

The gradient expansion and surface term.

The nuclear EOS.

The universal Energy Density Functional and NS structure

Conclusions and Prospects

THE EDF METHOD

e method is mainly based on the Hohenberg and Kohn theorem ,

ich proves the existence of a functional only of the density profile

at acquires its minimal value for the ground state density profile.

e value of the functional at the minimum is just the ground state energy

is functional gives the exact ground state density, and it is therefore

sentially unknown. It is expected to be non-local and of intricate structur

practical applications it is therefore assumed that it can be approximate

a simpler functional, which will provide an approximate density profile

d approximate energy of the ground state.

An explicit but simplified form of the functional is the Skyrme functional, which is based on an effective force.
It is adjusted to reproduce the ground state binding.

$$E = T + \frac{1}{2}\sum_{iklj} \rho_{ik} f^{A}_{il;kj}(\rho)\rho_{lj} = T + V(\rho)$$

$$\begin{aligned} < u\, s \,|\, \kappa \,|\, v\, t >_A &= \left(\frac{\delta^2 V}{\delta\rho_{st}\delta\rho_{uv}}\right)_0 \\ &= \tfrac{1}{2}\{\, f^{A}_{us;vt} + f^{A}_{su;tv} \\ &+ [\, \textstyle\sum_{lj} \left(\, \rho^0_{lj}\left(\frac{\delta f^{A}_{lu;jv}}{\delta\rho_{st}}\right) + \left(\frac{\delta f^{A}_{sl;tj}}{\delta\rho_{uv}}\right)\rho^0_{lj}\,\right) + \textstyle\sum_{iklj} \rho^0_{ik}\left(\frac{\delta^2 f^{A}_{il;kj}}{\delta\rho_{st}\delta\rho_{uv}}\right)\rho^0_{lj}\,]\} \end{aligned}$$

rearrangement term

The functional can be applied both to nuclear matter and finite nuclei

The simplest and most direct way to connect the infinite
homogeneous system and finite systems is to follow the
Kohn-Sham scheme.

One introduces a local density functional, that in the case of atoms and molecules reads

$$E[\rho] = T_s[\rho] + \int d\mathbf{r}\ v_{\rm ext}(\mathbf{r})\rho(\mathbf{r}) + E_H[\rho] + E_{\rm xc}[\rho]$$

$$E_H = \frac{e^2}{2} \int d\mathbf{r} \int d\mathbf{r}'\ \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

Besides the Hohenberg-Kohn theorem one assumes

- The exact functional can be approximated by a local one
- The density can be written

$$\rho(r) = \sum_i^A |\phi_i(r)|^2$$

Then

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{\rm eff}(\mathbf{r})\right)\phi_i(\mathbf{r}) = \epsilon_i\phi(\mathbf{r})$$

$$v_{\rm eff}(\mathbf{r}) = v_{\rm ext}(\mathbf{r}) + e^2\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + \frac{\delta E_{\rm xc}[\rho]}{\delta\rho(\mathbf{r})}$$

Iportant remark : the $\phi_i(r)$ are NOT the single particle levels orbitals

In particular the density matrix CANNOT be written as

$$\rho(r,r') = \sum_i^A \phi_i(r)^*\phi_i(r')$$

A further assumption is that the correlation energy is locally equal to the correlation energy of an electron gas at the local density.

This is a local density approximation, *which connects the functional with the bare particle interaction and many-body theory*.

The approximation can be improved by adding gradient corrections,

$$\nabla n, (\nabla n)^2, \nabla^2 n.......$$

The principle the expansion can be obtained from microscopic calculations in non-homogeneous gas, provided the density profile is smooth enough.

The key quantity is

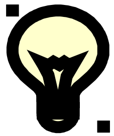
$$t = \nabla n / k_F \, n$$

Often used

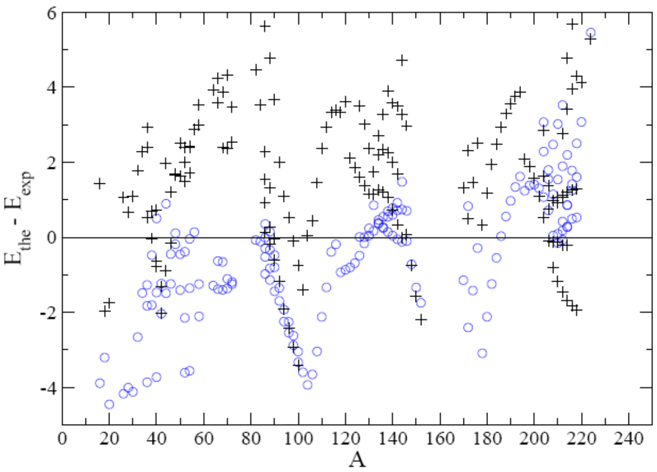
$$H = (e^2/a_0)\gamma\,\phi^3 \times \ln\left\{1 + \frac{\beta}{\gamma} t^2 \left[\frac{1 + At^2}{1 + At^2 + A^2 t^4}\right]\right\}$$

Predew et al. , PRL 77, 3865 (1996)

In nuclear physics it is not possible to separate the Hartree or Hartree-Fock term in the functional since the bare interaction has a strong repulsive core. One has then to include directly the whole EOS in the functional .



Density functionals from microscopic EOS !



Xavier advertising BCPM

EXOCT 2007

The nuclear Kohn-Sham functional can be then written

$$E = T_0 + E_N^{\mathrm{bulk}} + E_N^{\mathrm{surf}} + E_{\mathrm{coul}} + E_{\mathrm{s.o.}}$$

$$T_0 = \frac{1}{2m} \sum_{i,\sigma,q} \int |\nabla \varphi_i(\mathbf{r}, \sigma, q)|^2 d\mathbf{r}$$

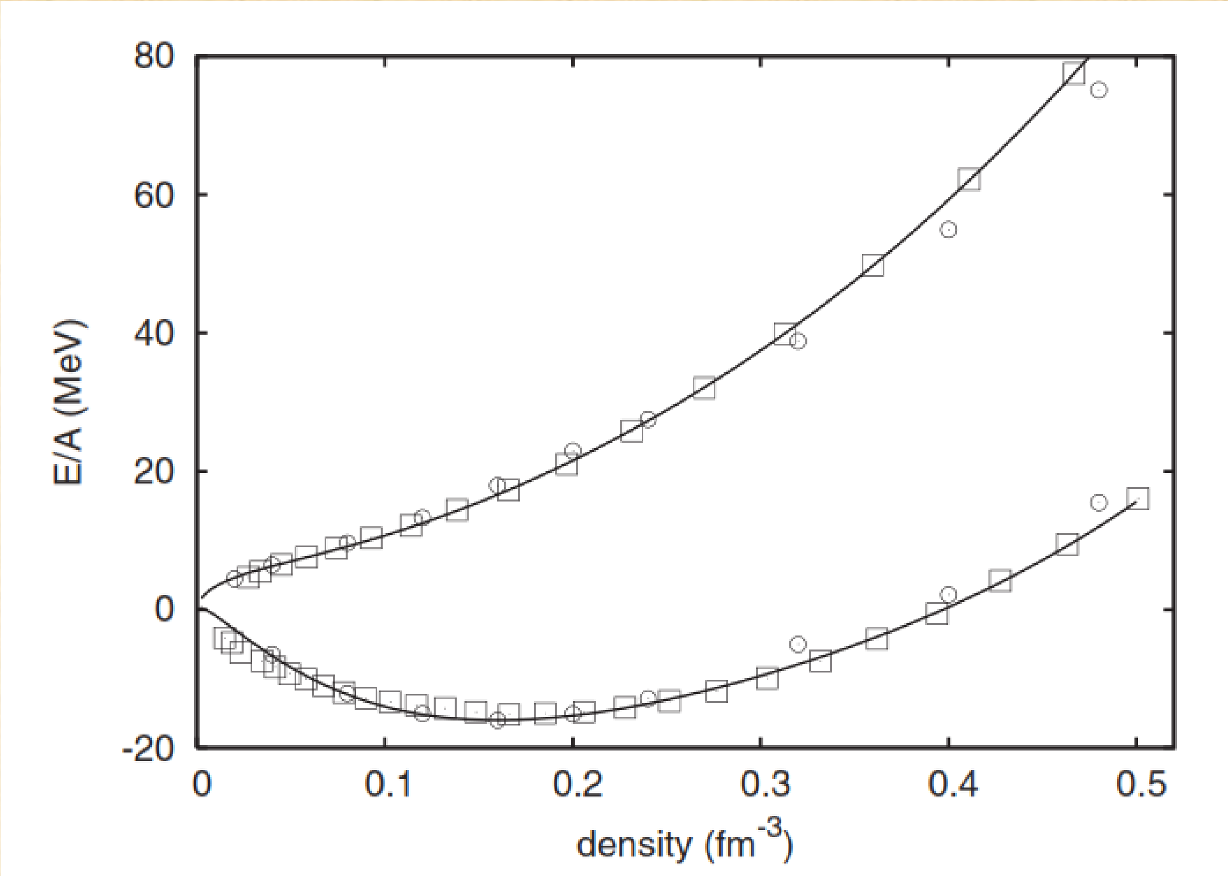
$$E_N^{\mathrm{surf}}[n_p, n_n] = \frac{1}{2} \sum_{q,q'} \int\int n_q(\mathbf{r}) v_{q,q'}(\mathbf{r} - \mathbf{r}') n_{q'}(\mathbf{r}') d\mathbf{r} d\mathbf{r}' - \frac{1}{2} \sum_{q,q'} \int n_q(\mathbf{r}) n_{q'}(\mathbf{r}) d\mathbf{r} \int v_{q,q'}(\mathbf{r}') d\mathbf{r}'$$

$$v_{q,q'}(r) = V_{q,q'} e^{-r^2/r_0^2}$$

← key quantity

The bulk part is taken from microscopic EOS.
The surface term is phenomenological.
The rest is standard

Bulk part from microscopic nuclear matter EOS



$$P(n) = \left(\frac{E}{A}\right) = \sum_{k=1}^{5} a_k \left(\frac{n}{n_0}\right)^k$$

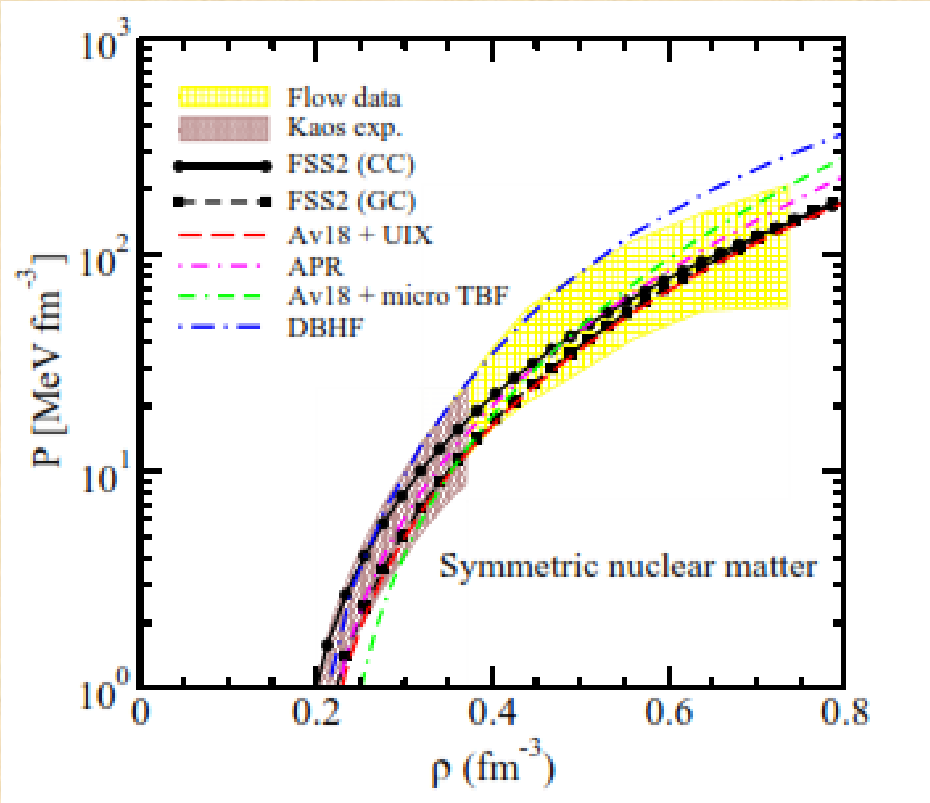
The coefficients are NOT parameters to be fitted to nuclear data.
They are fixed by the microscopic EOS

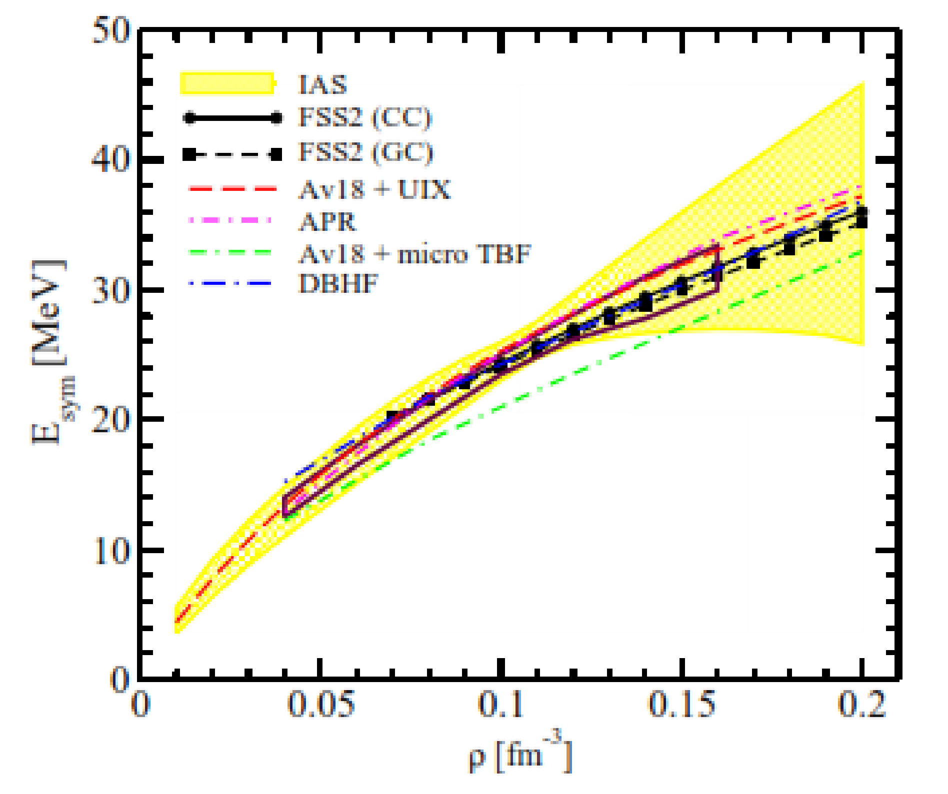
M. Baldo, L.M. Robledo,P.Schuck and X.Vinas, Phys. Rev. C87, The other physical characteristics of the EOS as obtained from the mcroscopic calculation.

Symmetry energy	J = 31.90 MeV
Slope of the S.E.	L = 52.96 MeV
Incompressibility	K = 212.4 MeV
Skewness	K’ = 879.6 MeV
Second derivative of J	KS = -96.75 MeV

These values are compatible with the ‘experimental’ constraints, with the possible exception of KS, which however is not well determined.

Other tests





Heavy ions

Nuclear structure : Symmetry energy

Some references

. Baldo, P. Schuck and X. Vinas, Phys. Lett. B663, 390 (2008)

M. Robledo, M. Baldo, P. Schuck and X. Vinas, Phys. Rev. C77, 051301 (2008)

Vinas, L.M. Robledo, P. Schuck and M. Baldo, Int. J. of Mod. Phys. E18, 935 (200

M. Robledo, M. Baldo, P. Schuck and X. Vinas, Phys. Rev. C81, 034315 (2010)

. Baldo, L.M. Robledo,P. Schuck and X. Vinas, J. of Phys. G 37, 064015 (2010)

. Baldo, L.M. Robledo,P.Schuck and X.Vinas, Phys. Rev. C87, 064305 (2013)

K. Sharma, M. Centelles, X. Vinas, G.F. Burgio and M. Baldo, A&A 584, A103 (20

. Baldo, L. Robledo, P. Schuck and X. Vinas, Phys. Rev. C95, 014318 (2017)

Since the BCPM functional by construction

can be applied both to nuclear matter and

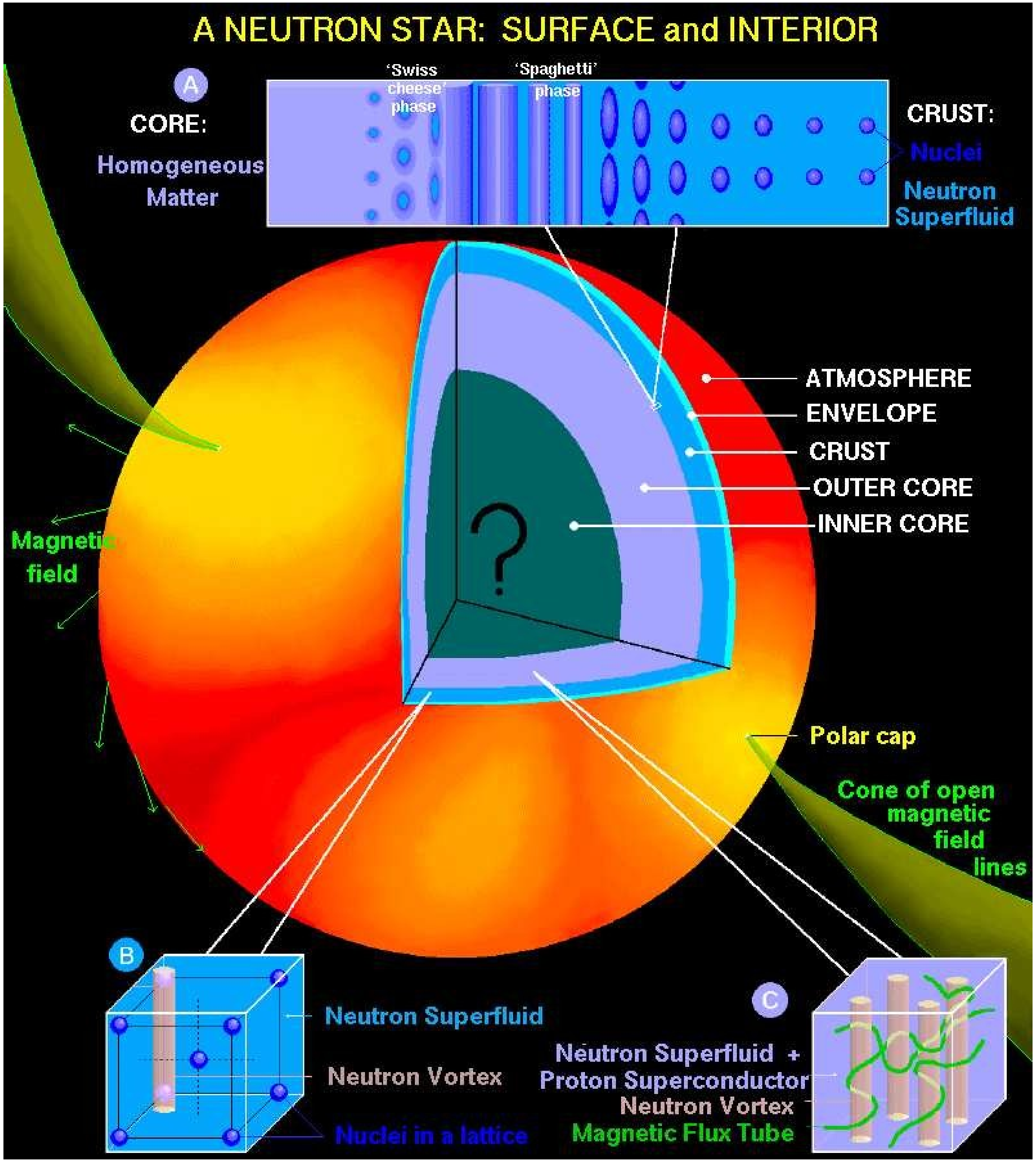
finite nuclei, it looks an ideal tool to study

the structure of Neutron Stars.

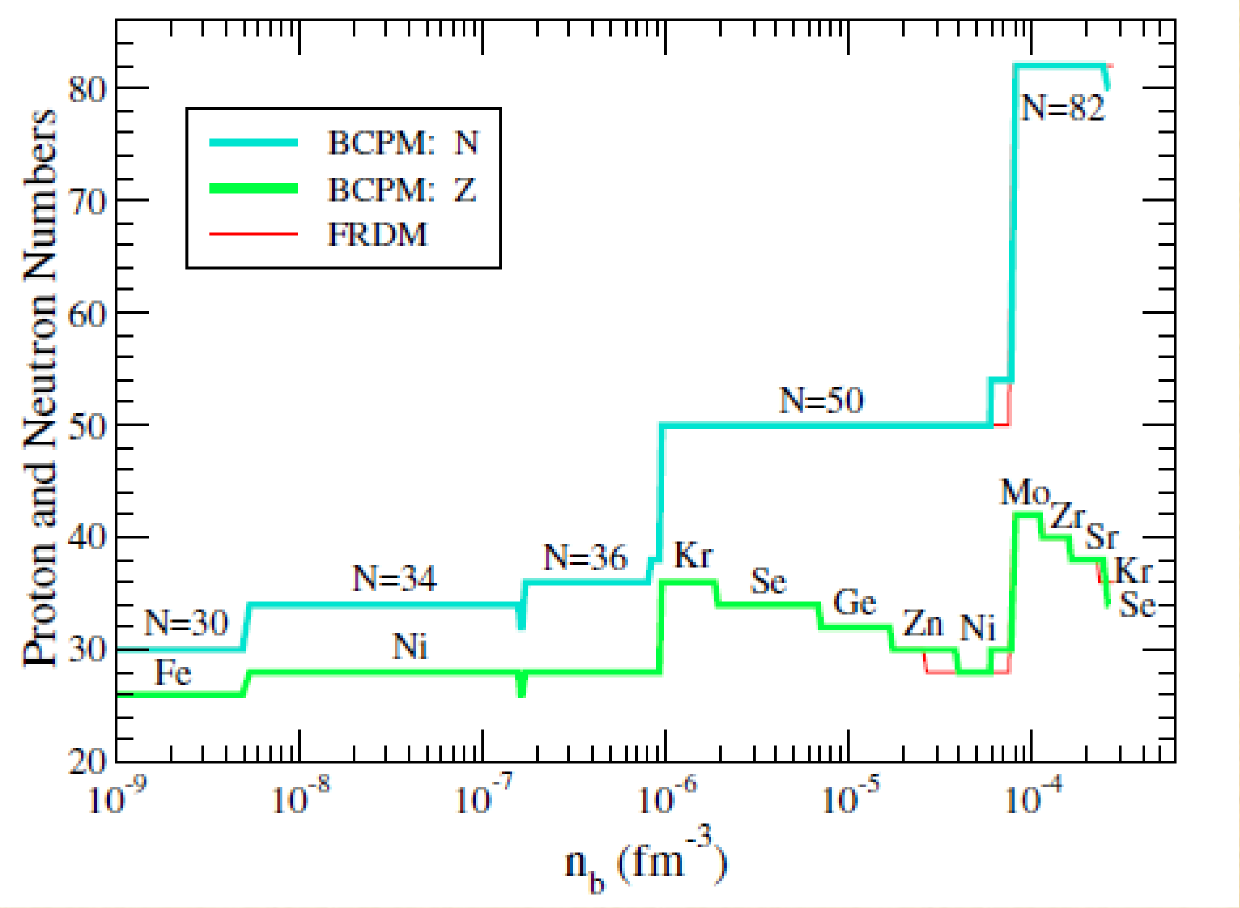
A section (schematic)

of a neutron star

Application of BCPM
to Astrophysics

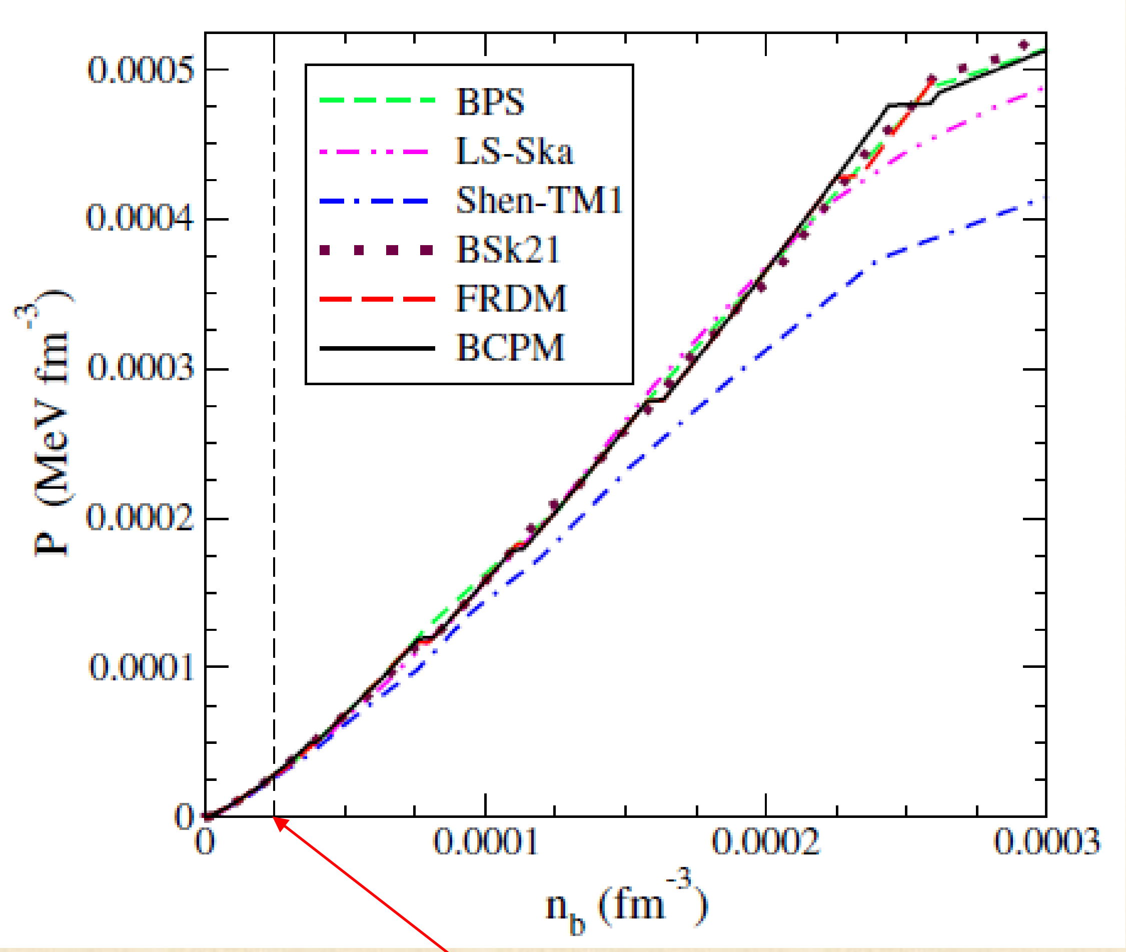


Outer crust composition from BCPM
Comparison with the Finite Range Droplet Model



B.K. Sharma, M. Centelles, X. Vinas, G.F. Burgio, M.B.
Astronomy & Astophysics 584, A103 (2015).

EOS of the outer crust
Comparison with more phenomenological model



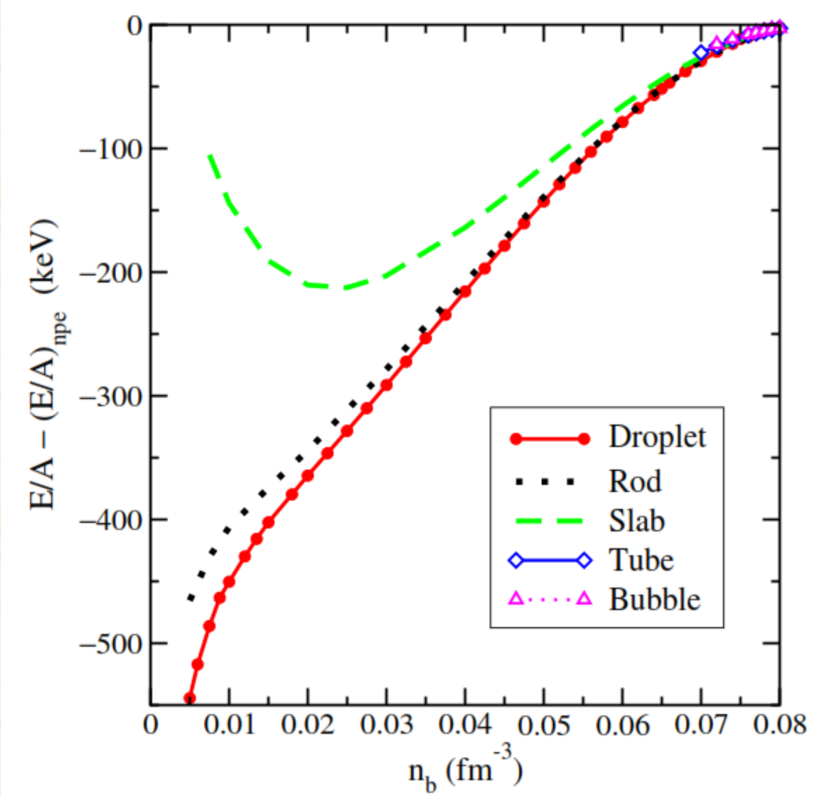
Limit of experimental data

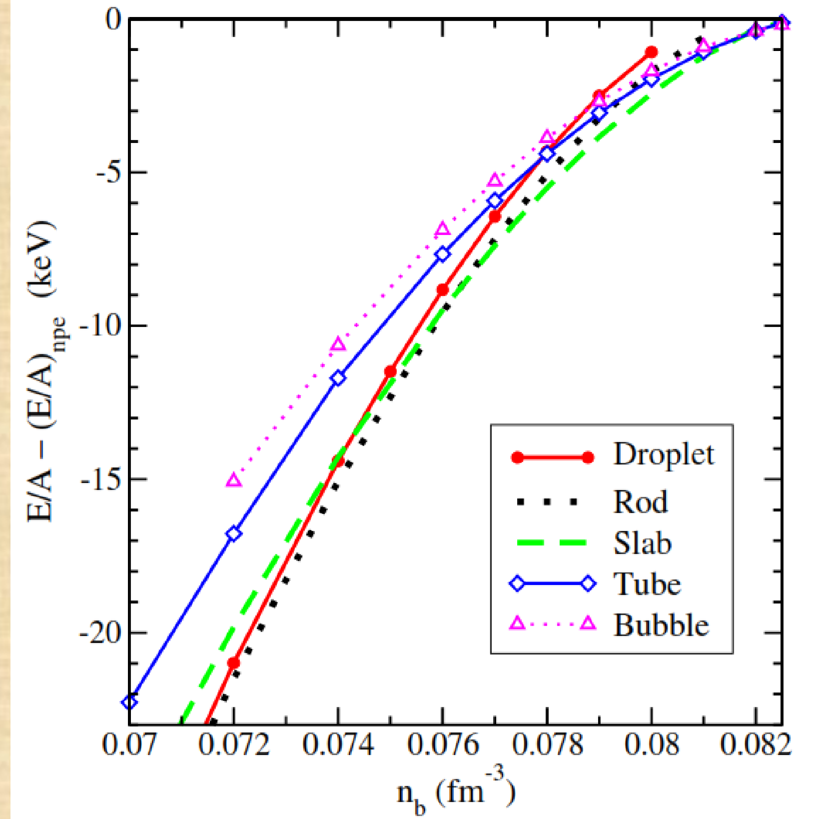
Inner crust

In the inner crust a series of shapes (‘ pasta phase ‘) are possible, besides the spherical one, which include a neutrona gas region.

Even within the Wigner-Seitz approximation, the full quantal calculations of the energy of these shapes is quite complex.

It is simpler (but still relatively complicated) to use an accurate Thomas-Fermi approximation.



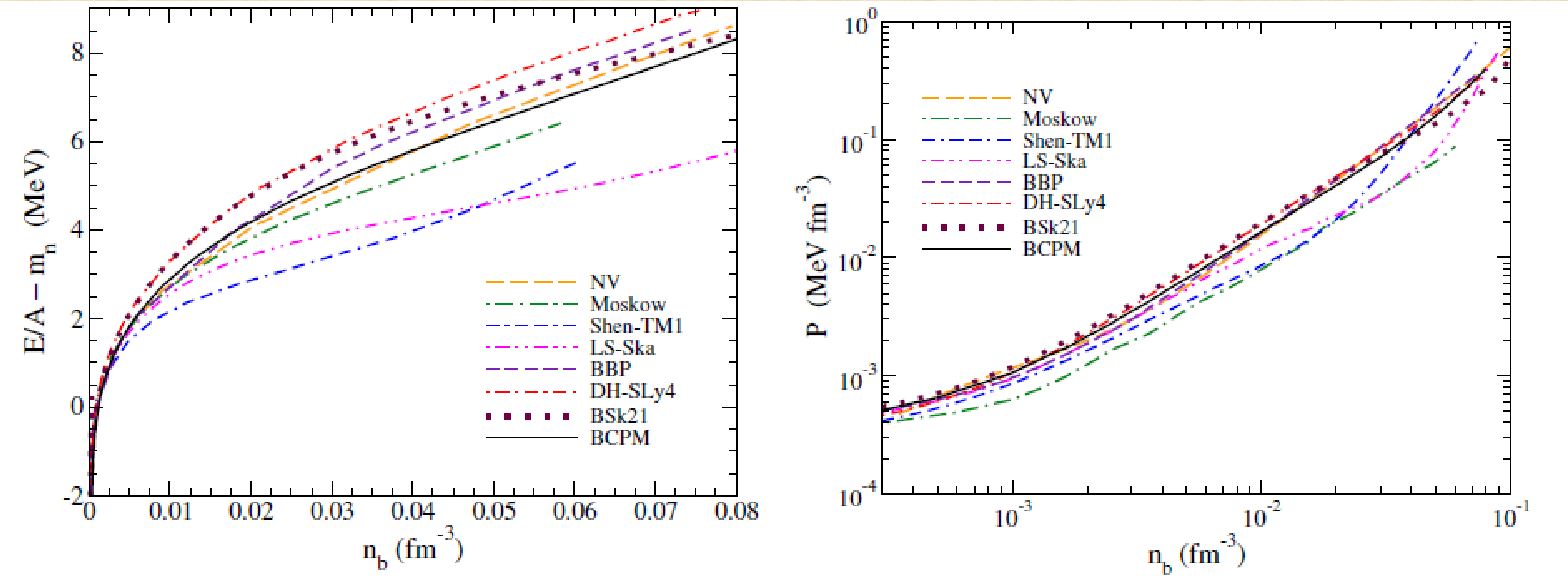


Structure of the Neutron Star inner crust
Physical conditions quite far from the laboratory ones

Tiny region for the genuine (non-spherical) ‘pasta’ phase

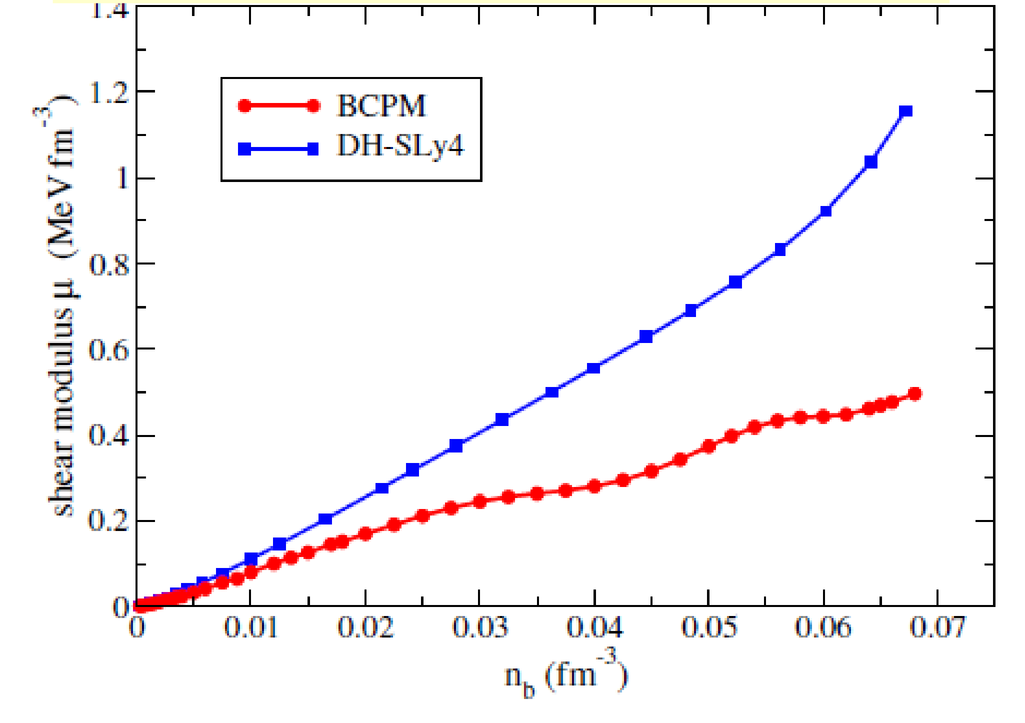
B.K. Sharma, M. Centelles, X. Vinas, G.F. Burgio, M.B.
Astronomy & Astophysics 584, A103 (2015).

Comparison with other EOS



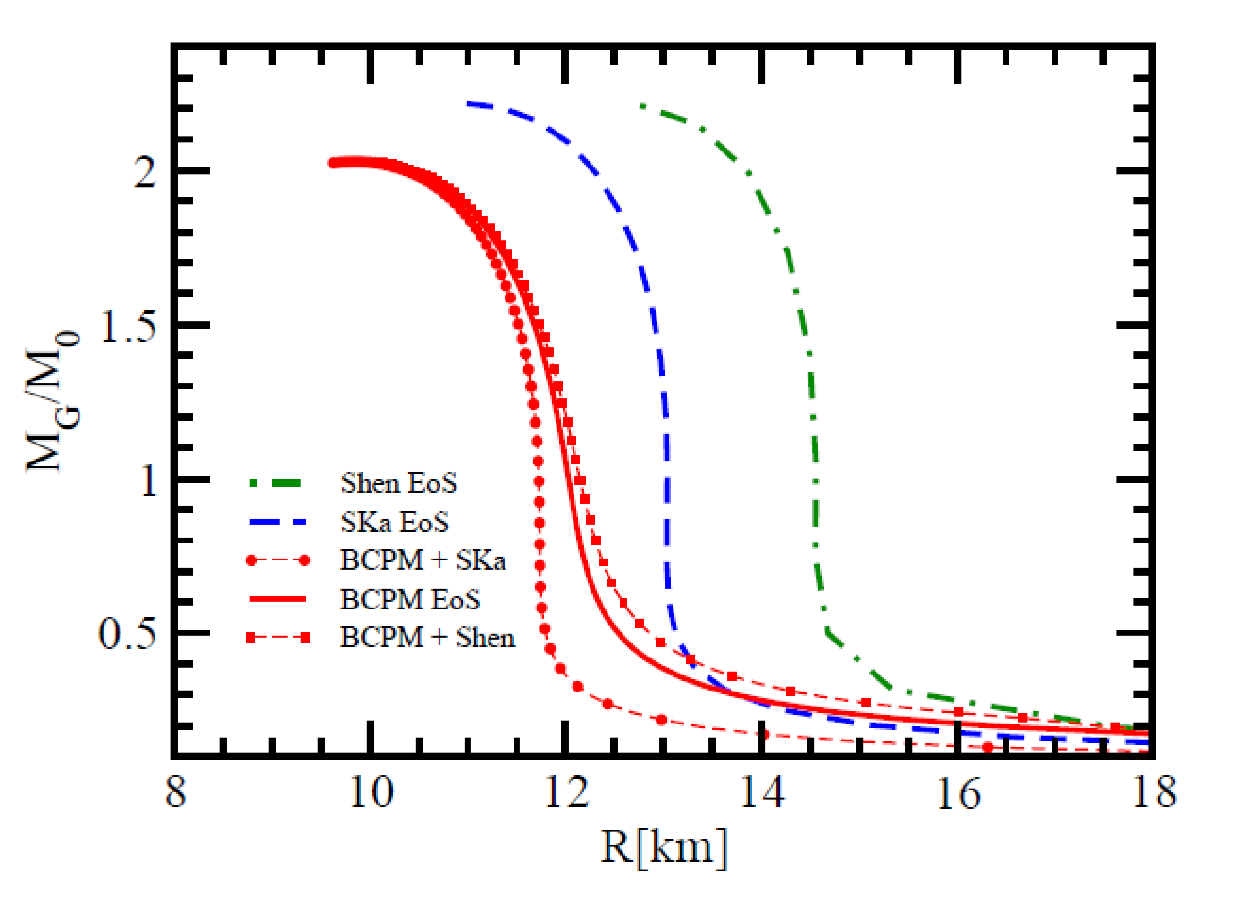
The difference in the EOS is expected to affect the inner crust properties.

Shear modulus of the crust



Oscillation frequencies → Z composition → symmetry energy

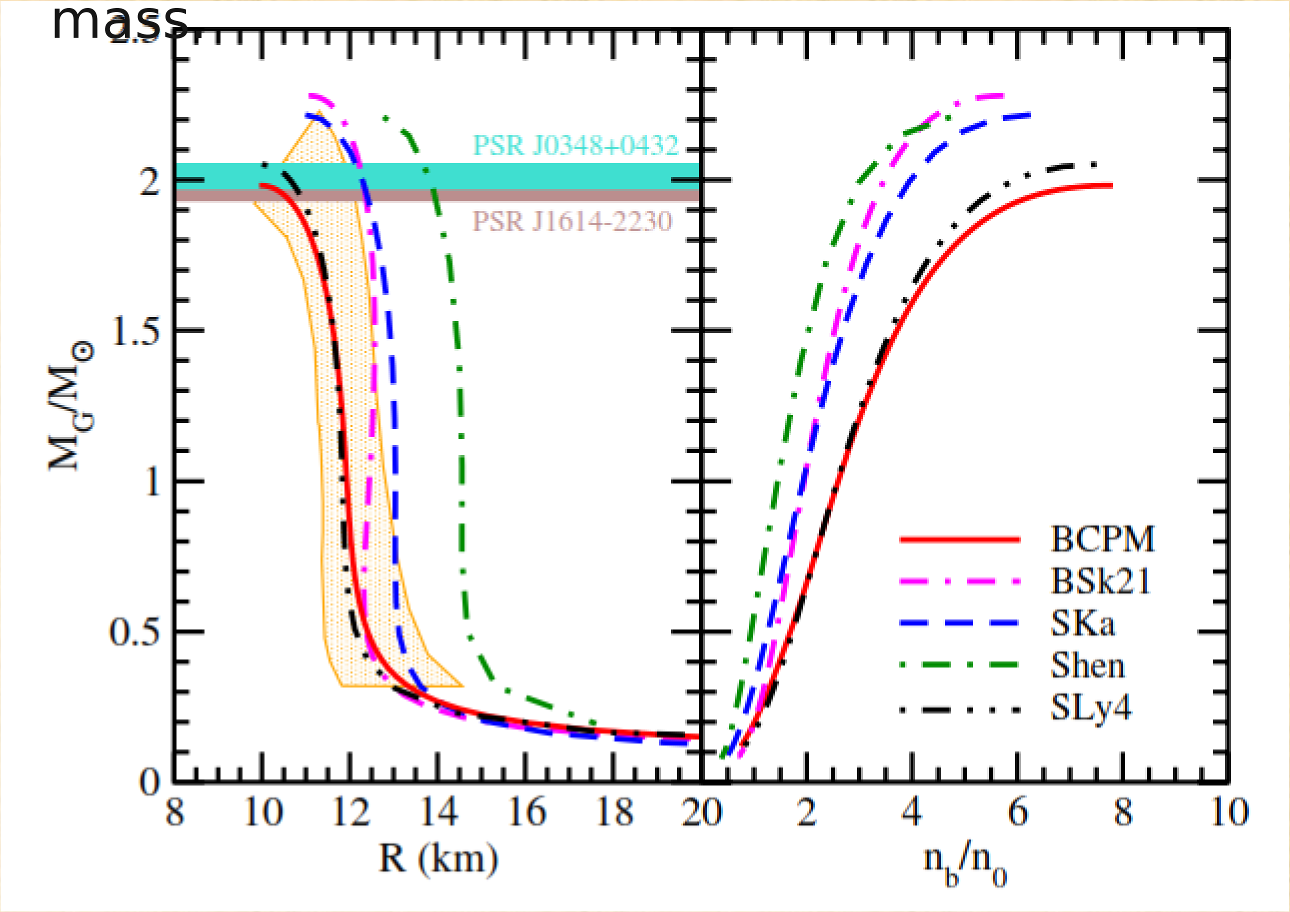
Relevance of the unified functional for the radius



Width of the crust

G.F. Burgio, M. Centelles, B.K. Sharma, X. Vinas, M.B.,
Phys. Atomic Nuclei 77, 1157 (2014).

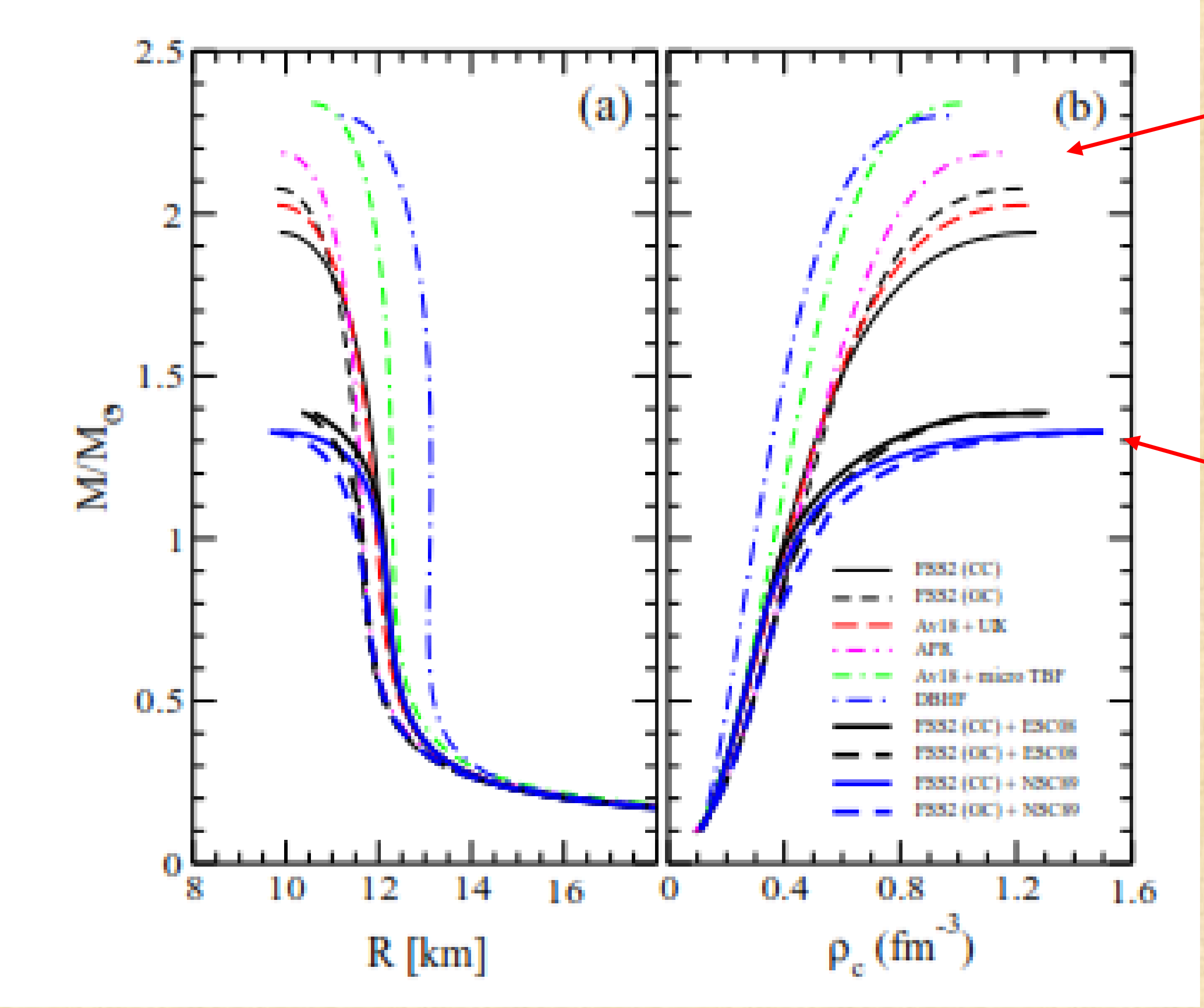
The constraint from the observed maximum mass.



The 2 solar mass constraint looks not so selective

B.K. Sharma, M. Centelles, X. Vinas, G.F. Burgio, M.B.
Astronomy & Astophysics 584 , A103 (2015)

Neutron Star mass as a function of radius and central density



Other (microscopic) EOS.

Dramatic effect of the hyperon component

Introducing quark matter

With respect to the MIT bag model there is need of additional repusion at high density.
This problem has been approached within several schemes

1. Color dielectric model

2. Nambu – Jona Lasinio model + additional interactions

3. Dyson – Schwinger equation

4. Field correlator method

5. Freedman & McLerran model of QCD

With a suitable choice of the parameters they are able to reach the two solar mass limit (but one must check that hyperons are prevented to appear or they have little effect)

CONCLUSIONS

The Kohn functional BCPM is based on a nuclear EOS
which is compatible with phenomenological constraints

It can be extended to include excited states

If one neglects ‘exotic’ components it is also compatible
with the observations on Neutron Stars masses

PROSPECTS

Other properties of NS (cooling, URCA, MURCA, transport ……).

In my end is my beginning

The joys of research in retirement

After retiring some ten years ago at the age of 65, I still wanted to do some worthwhile research (*Nature* **521,** 20–23; 2015).

I had only a chair and a table for support. These props came courtesy of my former employer, along with online access to the scientific literature. I was originally a researcher in two very different fields — surface science and nanoparticle-related health effects — so I set about re-evaluating publications in both areas. New ideas emerged, sparking successful collaborations with former

Xavier 2017 -----→

Nature 11-june-2015

BEST WISHES to Xavier
!