Fluctuations of the one-body distribution function

A. Bonasera, F. Gulminelli, and P. Schuck
Phys. Rev. C **46**, 1431 – Published 1 October 1992

ISN, Grenoble, 1993

Z. Phys. A – Hadrons and Nuclei 342, 397–401 (1992)

Zeitschrift für Physik A Hadrons and Nuclei

Wigner Kirkwood $\hbar$-expansion of the density matrix in inhomogeneous superfluid Fermi systems

K. Taruishi[1] and P. Schuck[2]

[1] Numazu College of Technology, 3600 Ooka, Numazu Shizuoka, 410 Japan
[2] Institut des Sciences Nucléaires, CNRS-JN2P3, Université Joseph-Fourier, 53, avenue des Martyrs, F-38026 Grenoble-Cédex, France

Received November 8, 1991

Clustering in the neutron star crust

F.Gulminelli, (LPC and Normandie Université, Caen)
with H.Dinh-Thi(LPC) and A.F.Fantina (GANIL)

Transport properties in compact stars

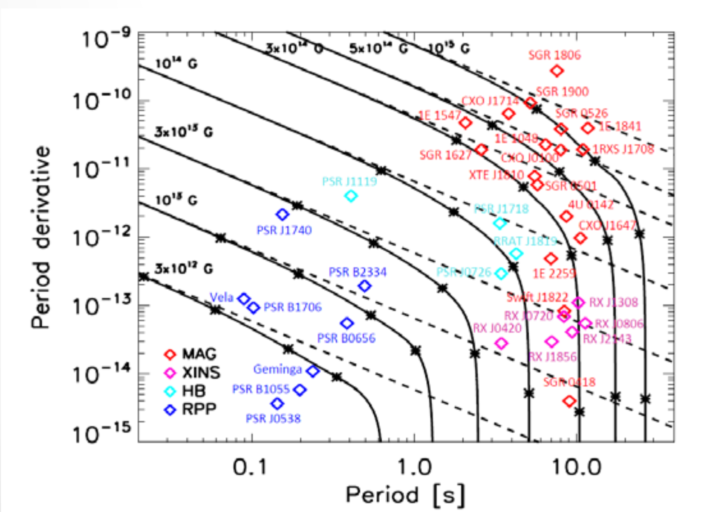
- Most signals from CS involve transport properties
- Some of them mainly concern $\rho \lesssim \rho_0$ matter ≡ clusters
  - NS cooling: B-thermal evolution
  - Relaxation after accretion & deep crust heating
  - CC, PNS cooling & mergers

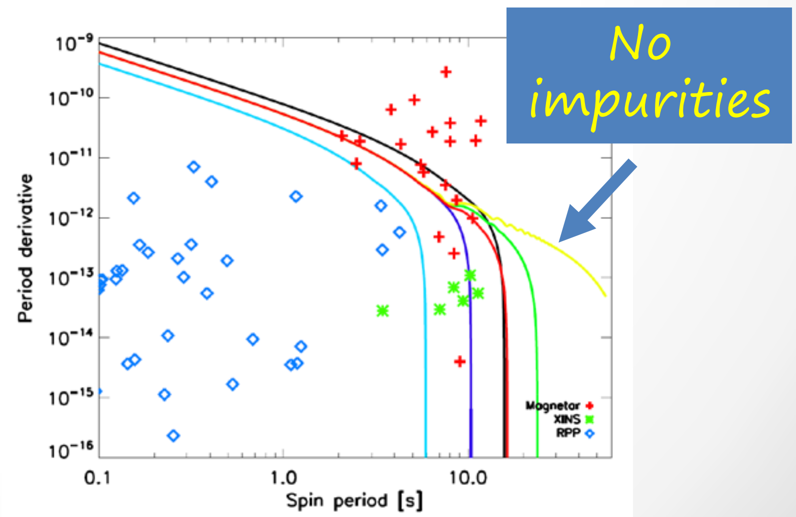
} e-Z, $T \approx 10^8 K$

ν-Z $T > 10^{10} K$

Schmitt&Shternin Springer 2018

- Key concept: quantify disorder => resistivity
  - T≫0 : distribution of nuclei (or pasta)
  - True even for a catalyzed crust: **impurities**





J.Pons et al. Nat.Phys. 2013

Transport properties in compact stars

- **$T<T_m$** $\quad \nu_{tot} = \nu_{e,i} + \nu_{e,imp}$ $\qquad Z^2 \leftrightarrow \boldsymbol{Q} = \sum_j \boldsymbol{n_j}\left(Z_j - \langle Z\rangle\right)^2$

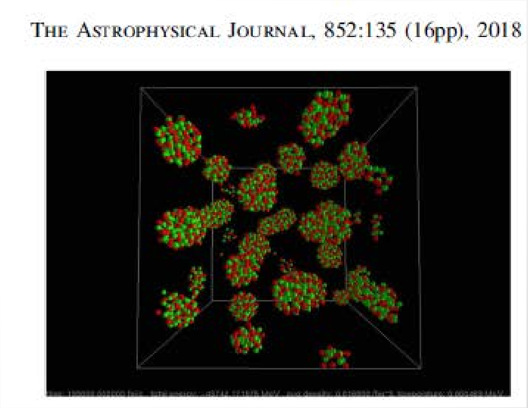
  Impurity factor
- **$T>T_m$** $\quad \nu_{e(\nu),i} \rightarrow \sum_j \boldsymbol{n_j} \nu^j_{e(\nu),i}$ $\qquad \nu^j_{e(\nu),i} \propto S^j(k)$

  Static structure factor

Present situation:

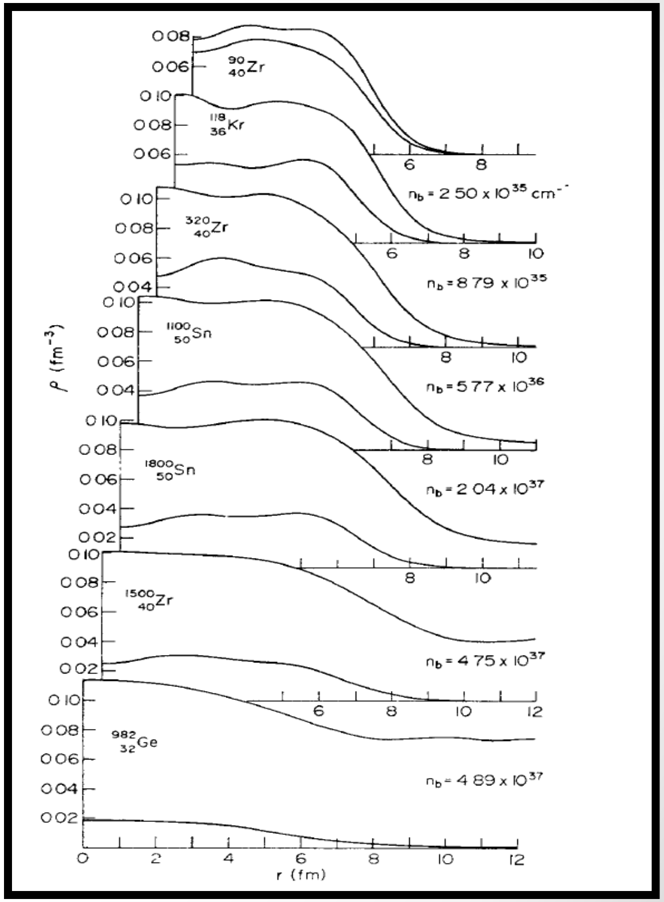
- Q taken as a free parameter in cooling and relaxation simulations *A.Deibel et al.ApJ839(2017)*
- n_j from Saha equations (Nuclear Statistical Equilibrium) or classical MD simulations *Z.Lin et al,PRC **102**(2020)045801*

$$n_{AZ} = g^T_{AZ}\left(\frac{M_{AZ}T}{2\pi\hbar^2}\right)^{3/2} exp\left[\frac{N\mu_n + Z\mu_p - M_{AZ}}{T}\right]$$



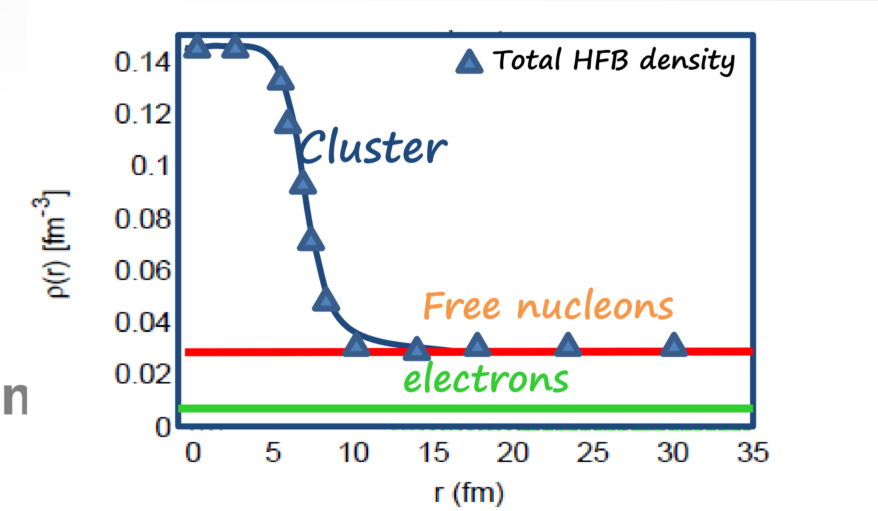
Towards a more controlled theoretical treatment

- Aim: having the nuclear functional as unique uncertainty ⇔ **unified** treatment at all ρ and T
- Let us start from what we know: variational calculations in the WS cell
- From WS cell to Multi-Component (liquid or solid) plasma: **cluster DoF**



J. W. Negele and D. Vautherin, NPA 207, 298 (1973)

From WS to MCP: mapping in 2 steps



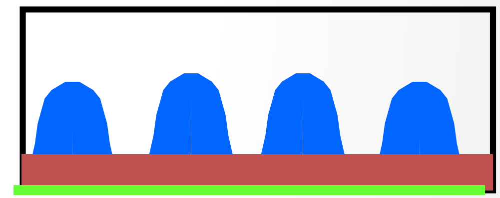
- **WS cell with a microscopic function** @(ρ_B, Y_p, T):

$$\mathcal{F}_{WS}\left(\hat{\rho}_q, \hat{\kappa}_q\right) = \mathcal{E}_{micro} - TS_{micro} = min$$

=> *Optimal particle (and pairing) densities*

1. OCP with cluster DoF

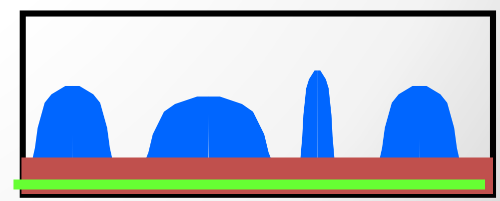
$$\mathcal{F}_{WS} \equiv \mathcal{F}^{OCP}(A, Z, \rho_{gq}) = \mathcal{F}(\rho_{gq}) + \frac{F_{AZ}}{V_{WS}} = min$$



=> *Optimal cluster*

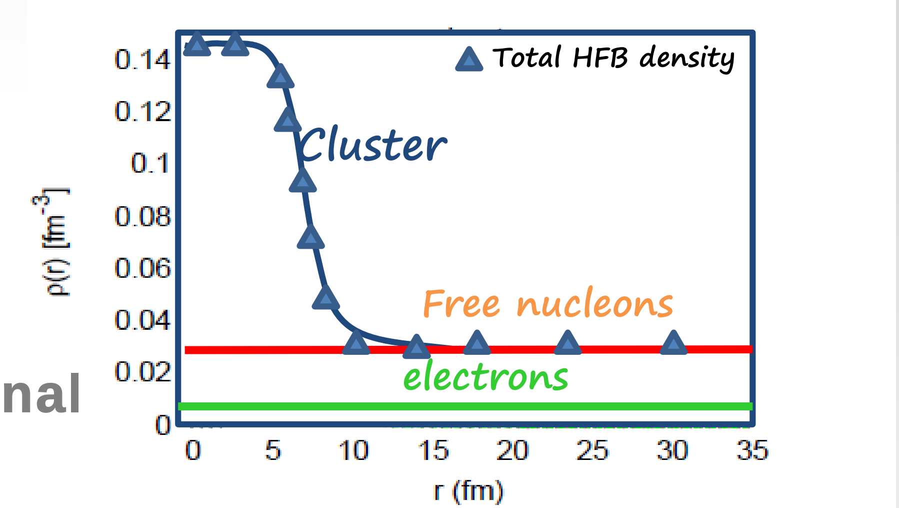
2. MCP with cluster DoF

$$\mathcal{F}^{MCP}(\{n_{AZ}\}, \rho_{gq}) = \mathcal{F}(\rho_{gq}) + \sum_{A,Z} n_{AZ} F_{AZ} = min$$



=> *Optimal distribution*

From WS to MCP: mapping in 2 steps



- **WS cell with a microscopic functional** $@(\rho_B, Y_p, T)$:

$$F_{AZ} = V_{WS}(\mathcal{F}_{WS} - \mathcal{F}_g) + \mathcal{F}_g V_{AZ} + \delta F$$

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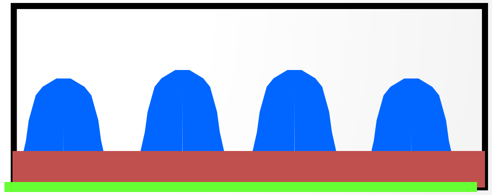

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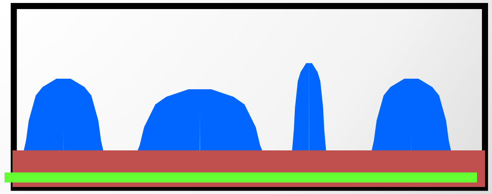
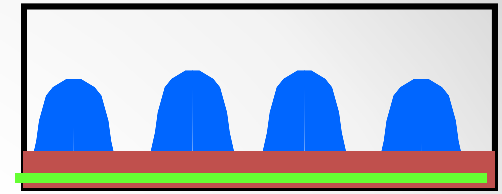


=> Optimal distribution

OCP with cluster DoF



$$\mathcal{F}^{OCP}(A, Z, \rho_{gq}) = \mathcal{F}(\rho_{gq}) + \frac{F_{AZ}}{V_{WS}} \approx \mathcal{F}_{WS}$$

- Below drip: F_{AZ} is just the HFB free energy
- Above drip: $F_{AZ}(A, Z, \rho_{gq})$

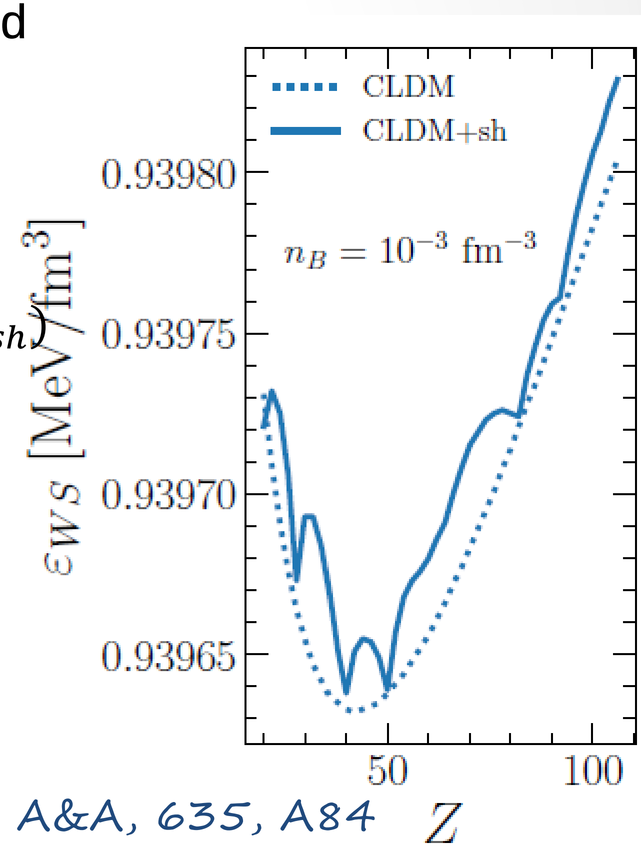
⇒ the cluster functional is in-medium modified

⇒ Practical implementation: F_{AZ} parametrized as a CLDM with surface parameters fitted from TETF calculation

$$F_{AZ}^{0} = V_{AZ}\left(\mathcal{F}(\rho_{bulk,q}) - \mathcal{F}(\rho_{gq})\right) + F_{surf} + F_{coul}(+F_{sh})$$

Continuum subtraction

Tubbs&Koonin, ApJ 232 (1979) L59
Bonche,Levit,Vautherin NPA427(1984)278



Carreau 2020, A&A, 635, A84

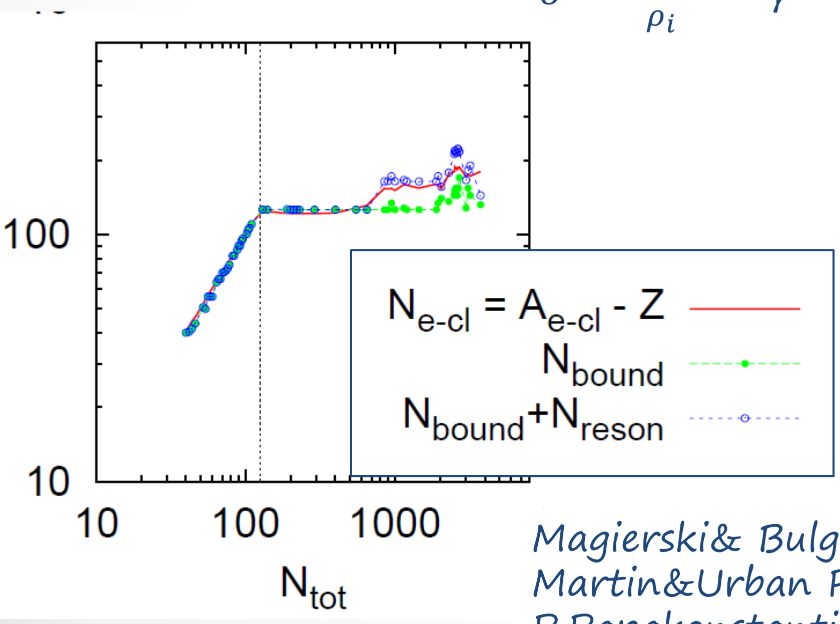
OCP with cluster DoF

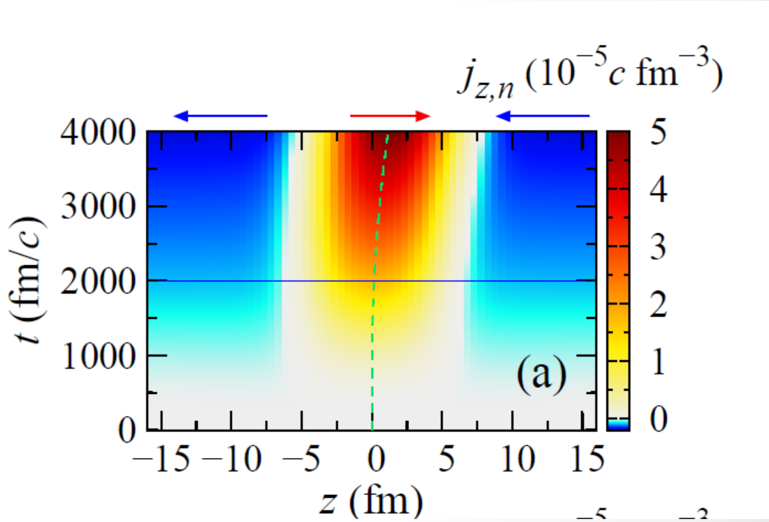
$$F_{AZ} = F^0_{AZ} + T\left(ln \frac{\lambda^3_{AZ}(M^*)}{gV_f} - 1 \right)$$

- CM degree of freedom: translation ($T>T_m$)
- n-p interaction: (only) bound neutrons are entrained by the ion

$$M^* = M\left(1 - \delta^f + \frac{(\delta^f - \gamma)^2}{\delta^f + 2\gamma}\right) \approx M\left(1 - \frac{\rho_{gn}}{\rho_i}\right)$$

$$\delta^f = \frac{\rho^f_n}{\rho_i} \qquad \gamma = \frac{\rho_{gn}}{\rho_i}$$





K.Sekizawa et al PRC 2022

Magierski& Bulgac NPA 2004
Martin&Urban PRC 2016
P.Papakonstantinou et al, PRC 2013

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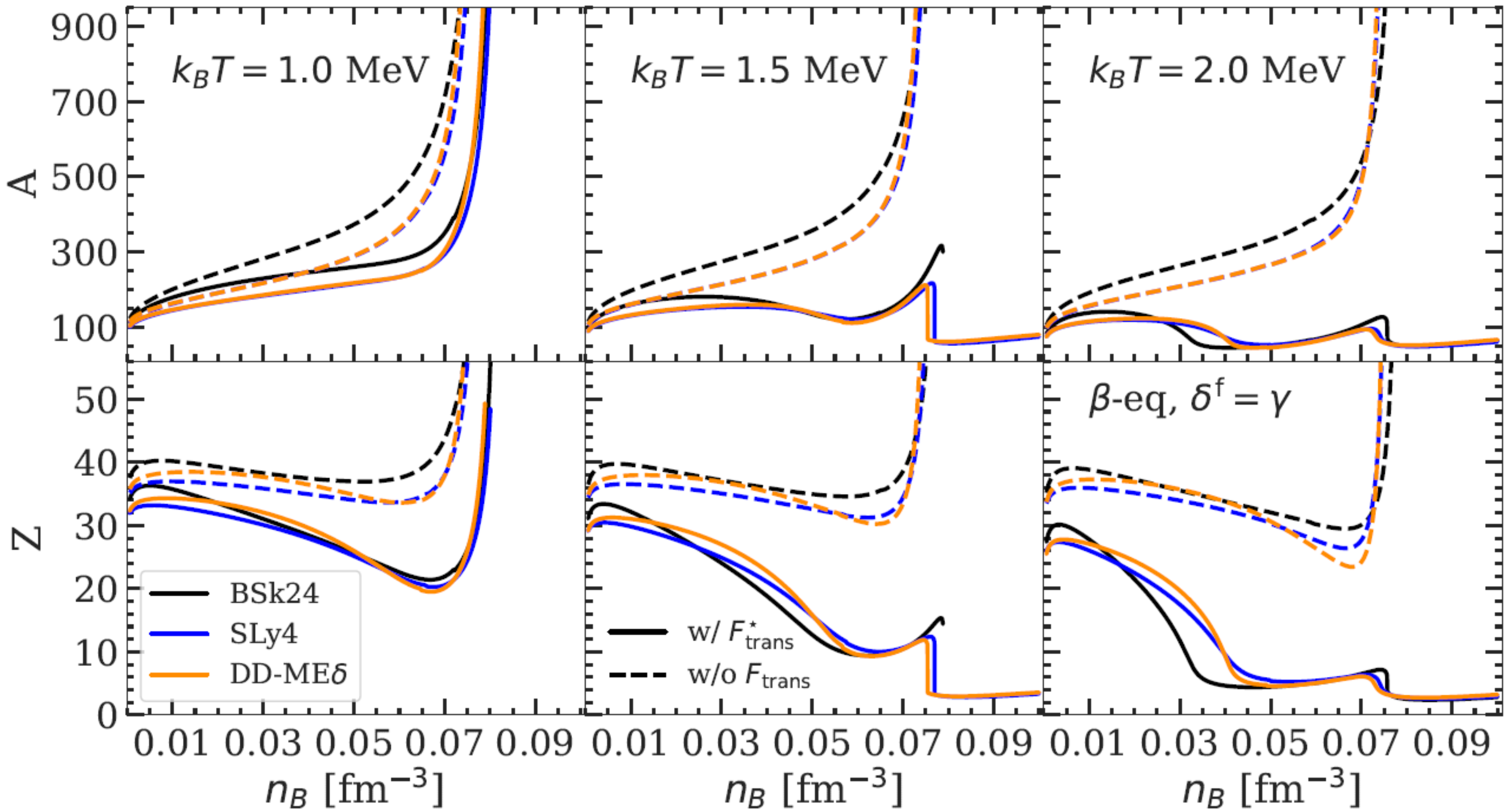
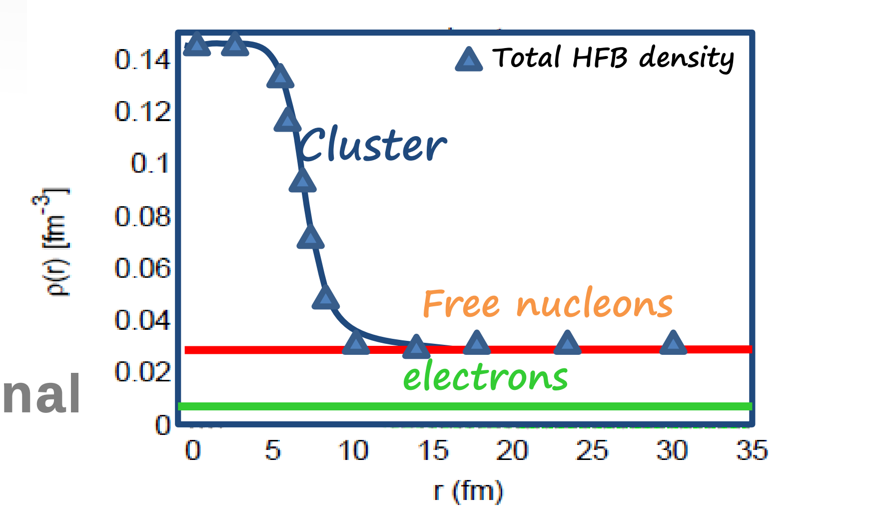


Essentially He clusters
@high density !

H.DinhThi et al, A&A in press

From WS to MCP: mapping in 2 steps



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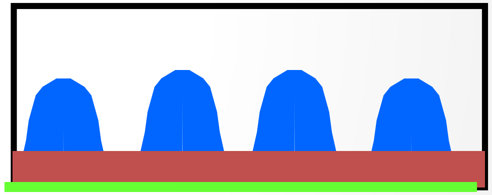
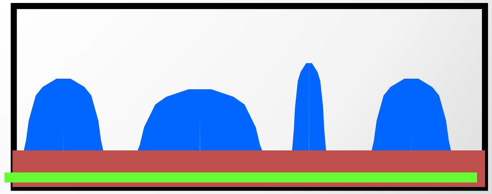


=> Optimal cluster

2. **MCP with cluster DoF**

$$\mathcal{F}^{MCP}(\{n_{AZ}\}, \rho_{gq}) = \mathcal{F}(\rho_{gq}) + \sum_{A,Z} n_{AZ} F_{AZ} = min$$

=> Optimal distribution



The cluster distribution

Grams 2018, PRC, 97, 035807
Fantina 2020, A&A, 633, A149
Carreau 2020, A&A, 640, A77
Dinh-Thi 2023, to be submitted

- $d\mathcal{F}_{MCP}(\{n_{AZ}\}) = 0$ leads to:

Continuum subtracted & microscopic level density

$$n_{AZ} = \left(\frac{M^*_{AZ} T}{2\pi\hbar^2}\right)^{3/2} \exp\beta\left[N\mu_n + Z\mu_p - F_i + R_{AZ}(n_e)\right]$$

Rearrangement $(n_e = \sum_{AZ} Z n_{AZ})$

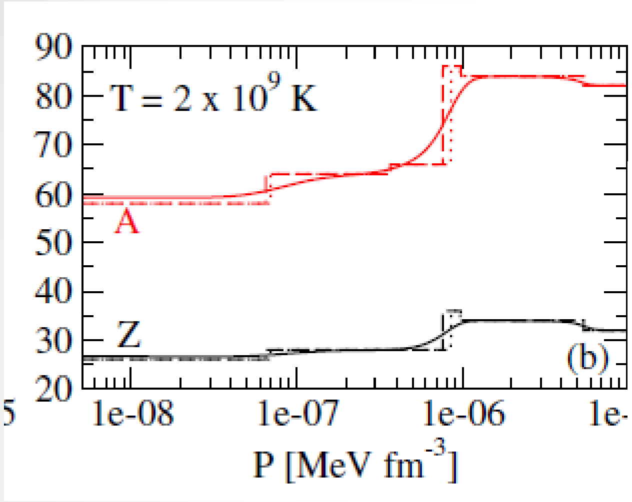
$$\mu_q = \frac{\partial \mathcal{F}_\mu}{\partial \rho_{gq}} + \sum_{AZ} n_{AZ} \frac{\partial F_{AZ}}{\partial \rho_{gq}} \left(1 - \sum_{AZ} n_{AZ} V_{AZ}\right)^{-1} \approx \frac{\partial \mathcal{F}_\mu}{\partial \rho_{gq}} + \frac{1}{V_{WS}^{OCP}} \frac{\partial F_{AZ}^{OCP}}{\partial \rho_{gq}} \left(1 - u_{AZ}^{OCP}\right)^{-1}$$

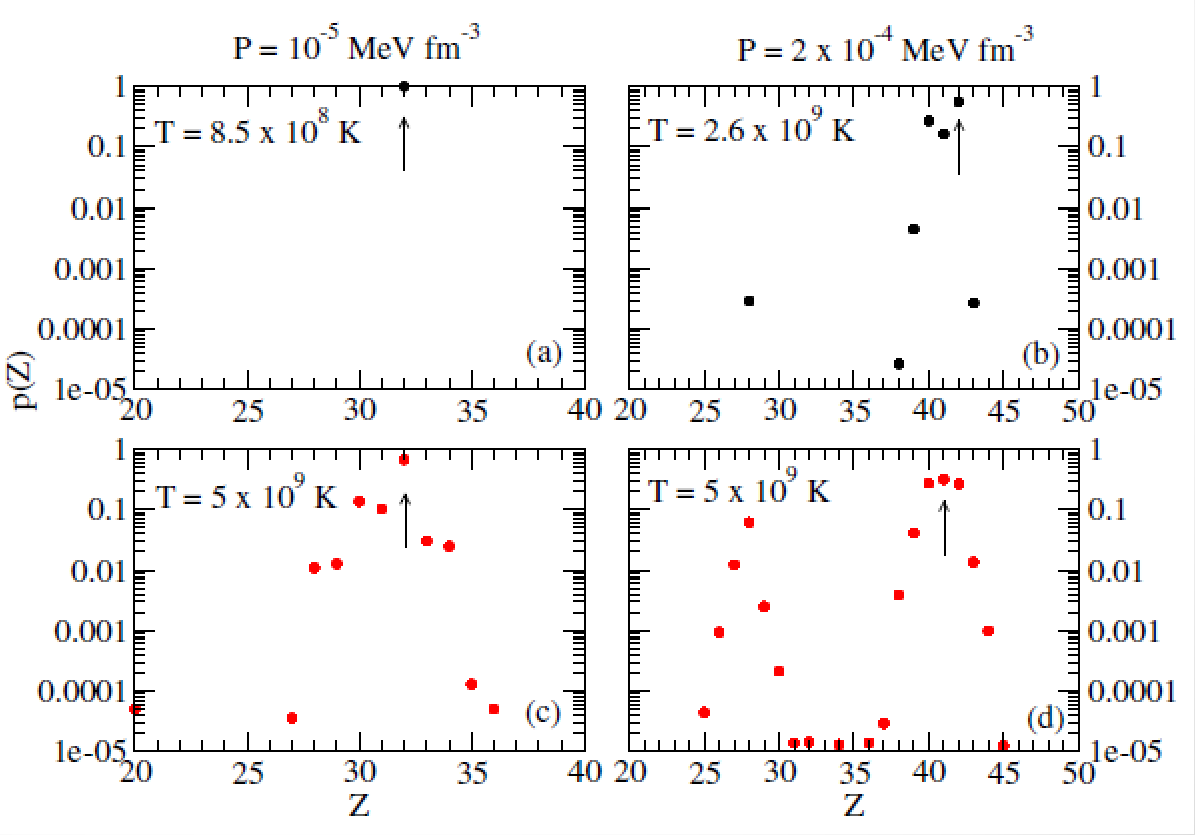
$$= \mu_q^{OCP}$$

Self-consistent $\mu(\rho)$

Perturbation 1st order

Nuclear distribution in the outer crust





Fantina 2020, A&A, 633, A149

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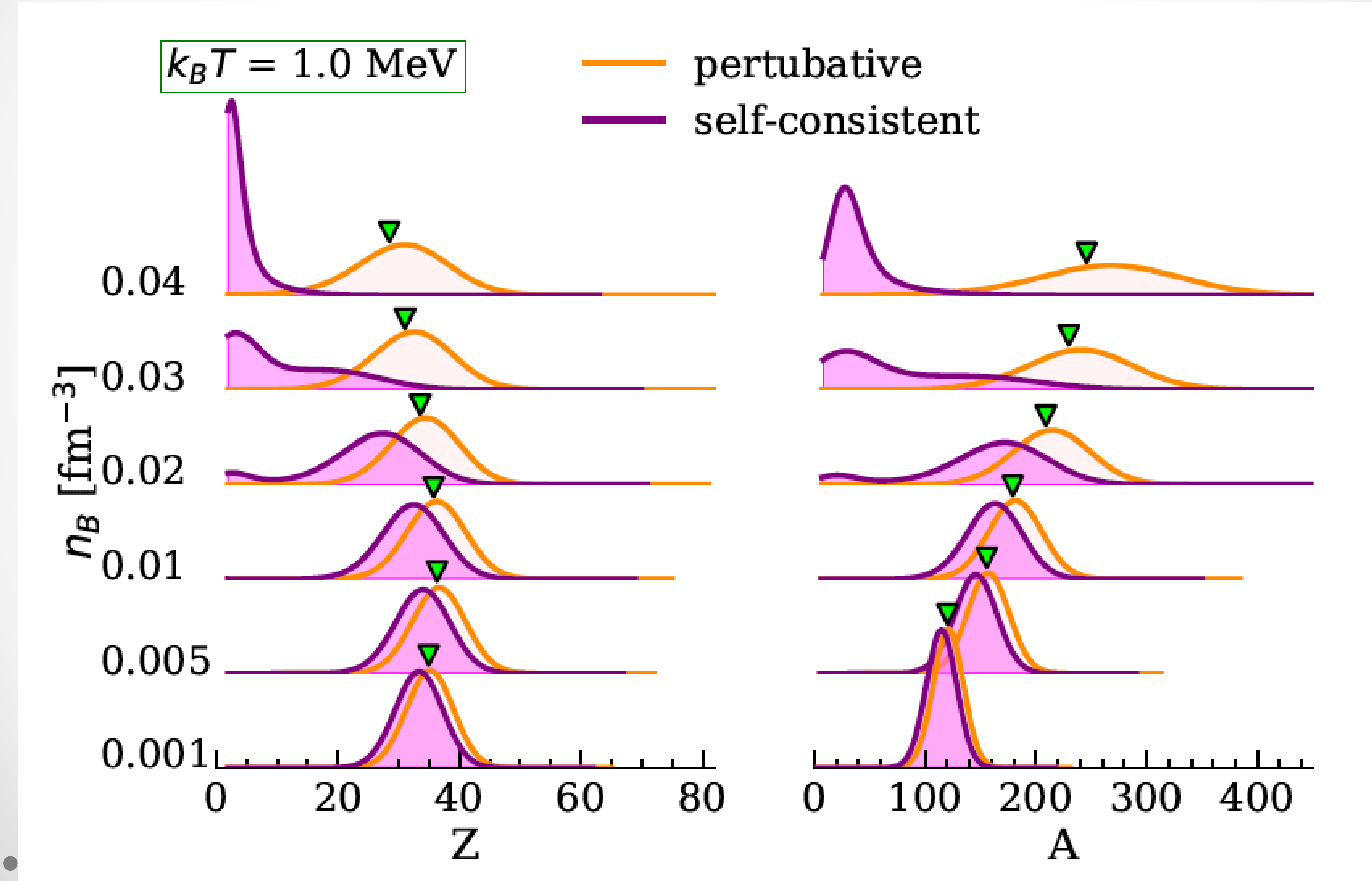
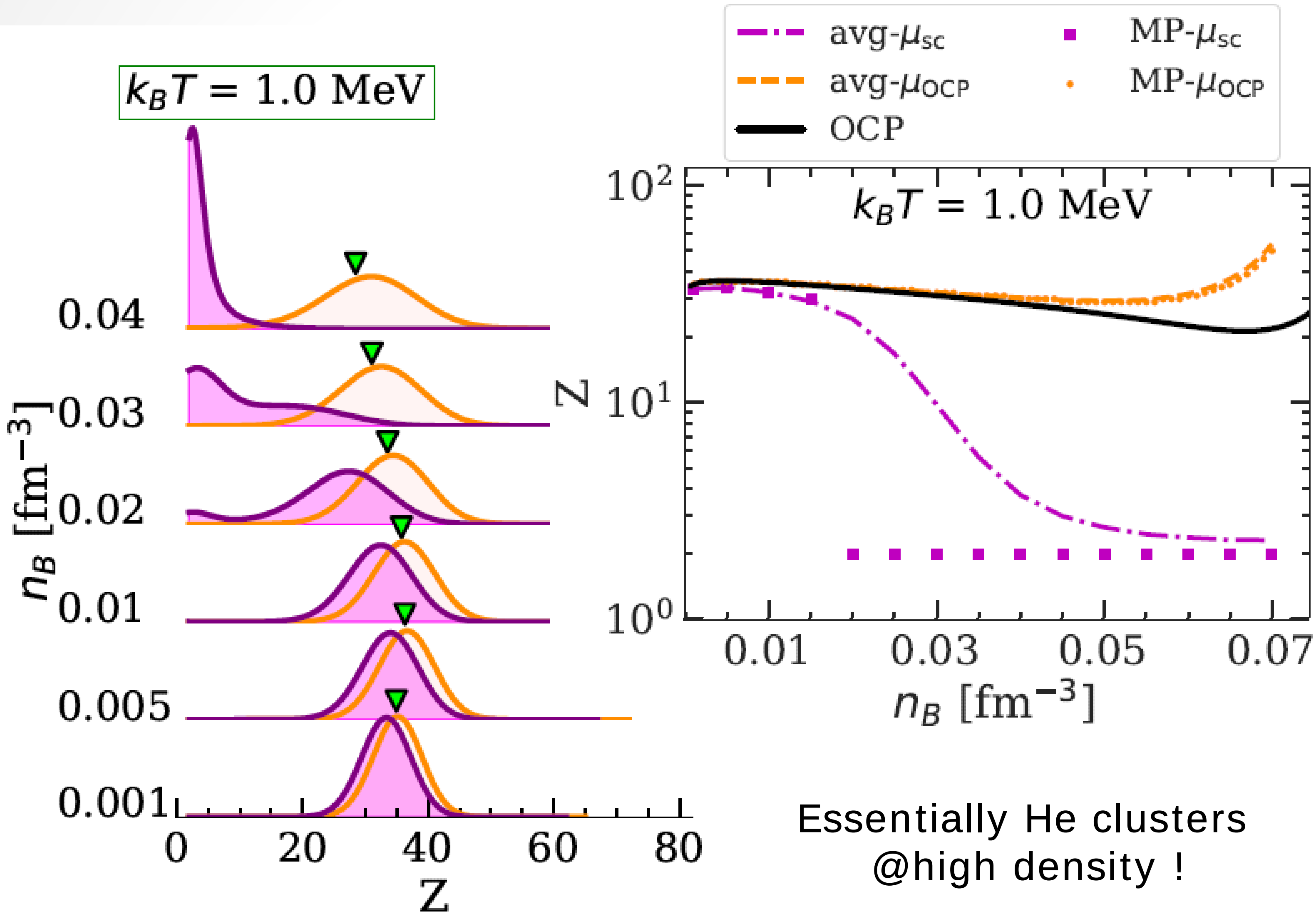
Dinh-Thi 2023, to be submitted



The cluster distribution

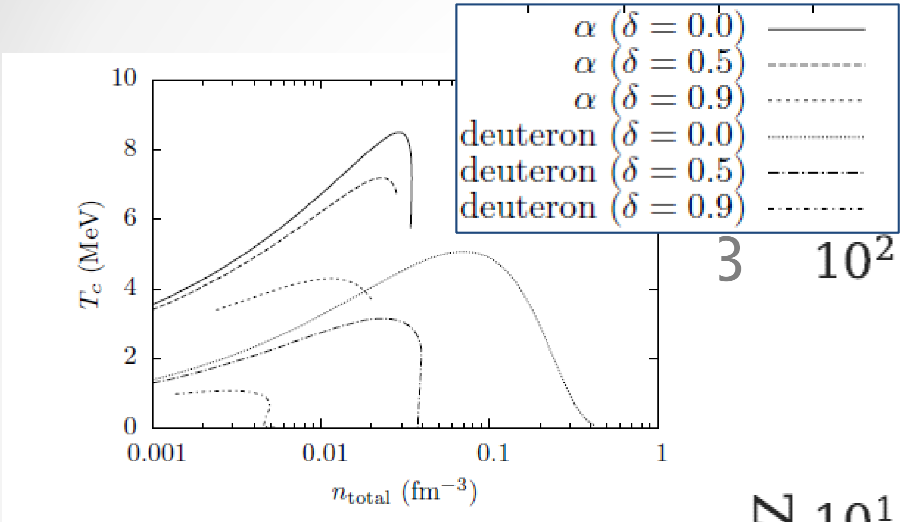
Dinh-Thi 2023, to be submitted



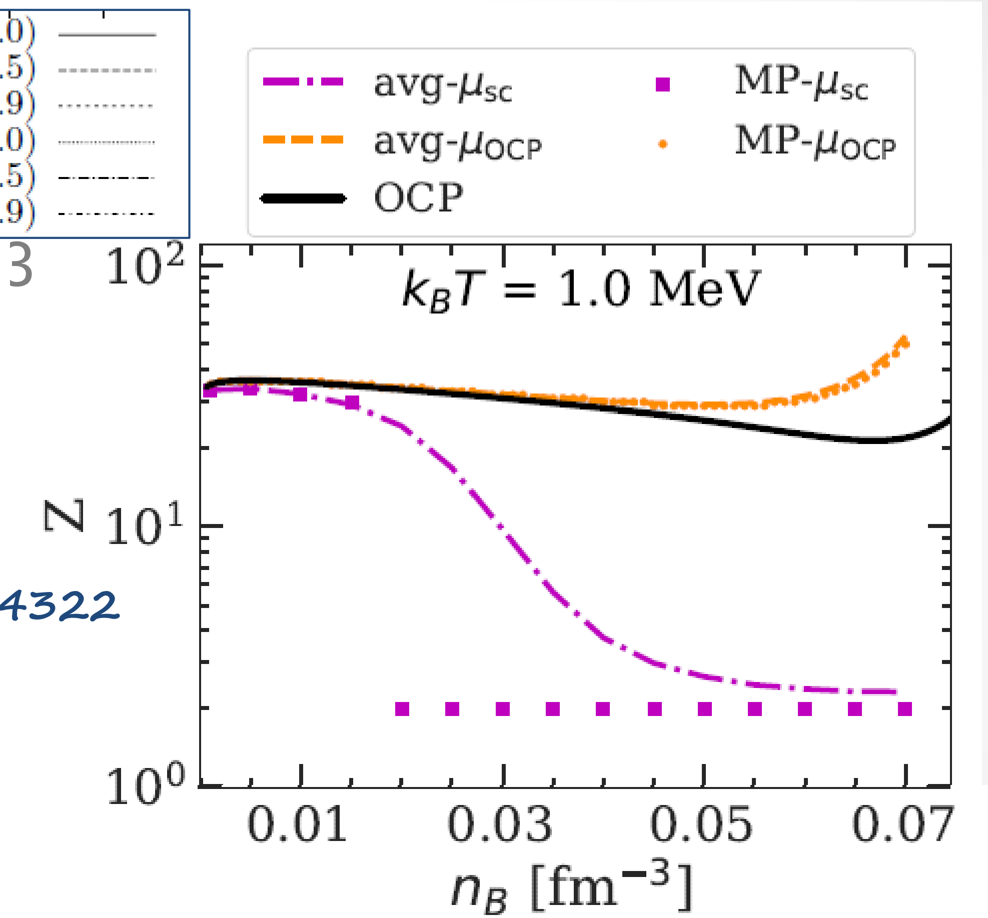
Essentially He clusters
@high density !

The cluster distribution

Dinh-Thi 2022, to be submitted



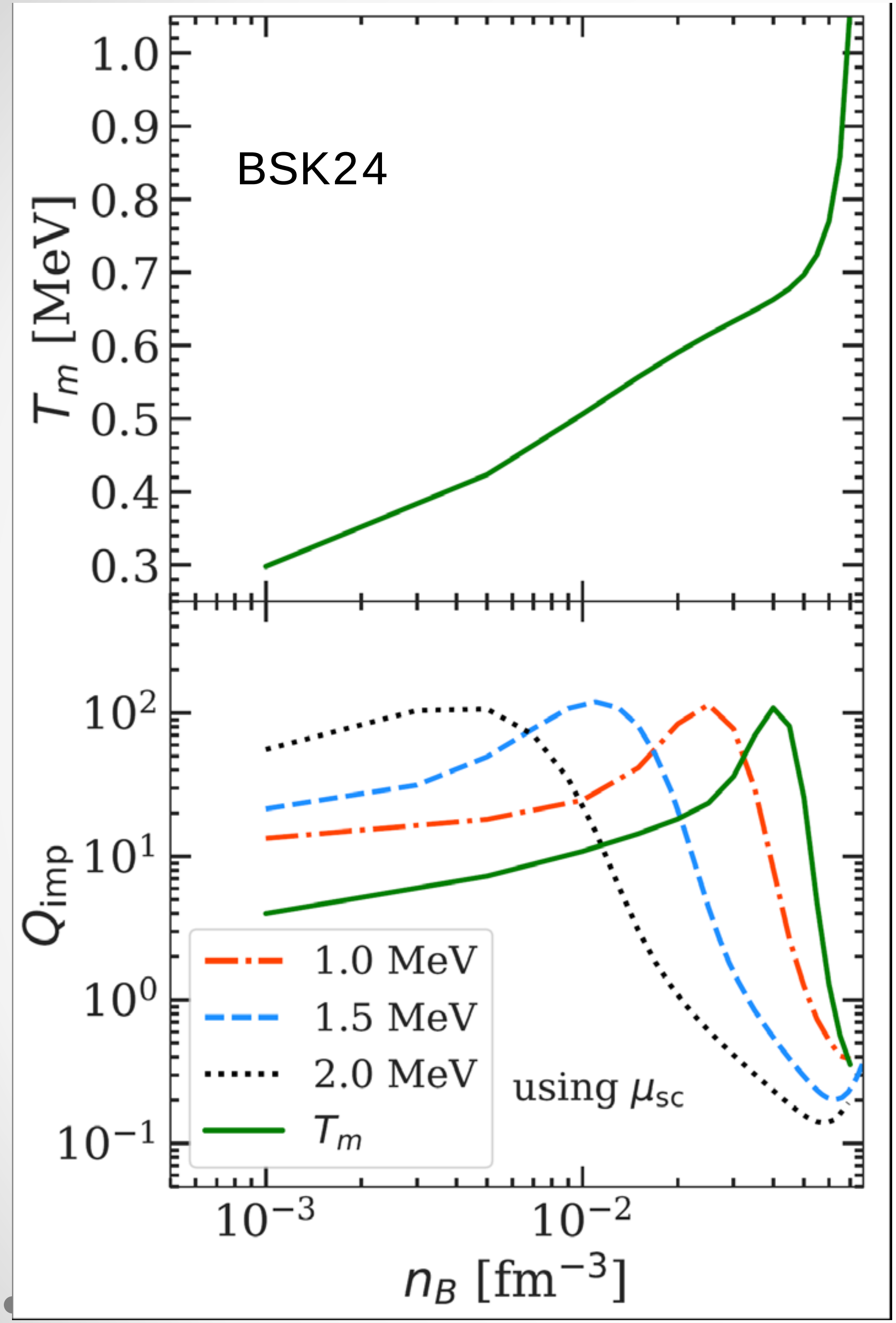
Takaaki Sogo, Gerd Röpke, and Peter Schuck, Phys. Rev. C 82, 034322

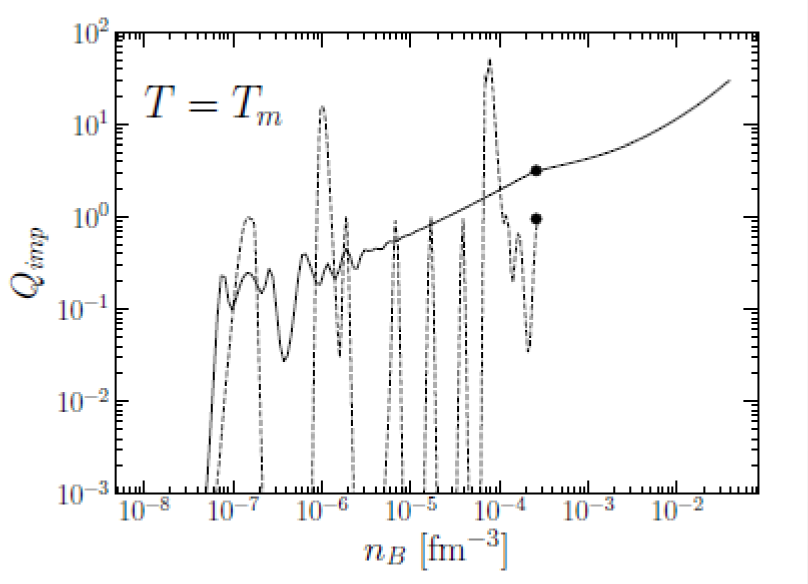


Essentially He clusters @high density !

Impurity factor

$$Q = \sum_j n_j \left(Z_j - \langle Z \rangle\right)^2$$





Conclusions

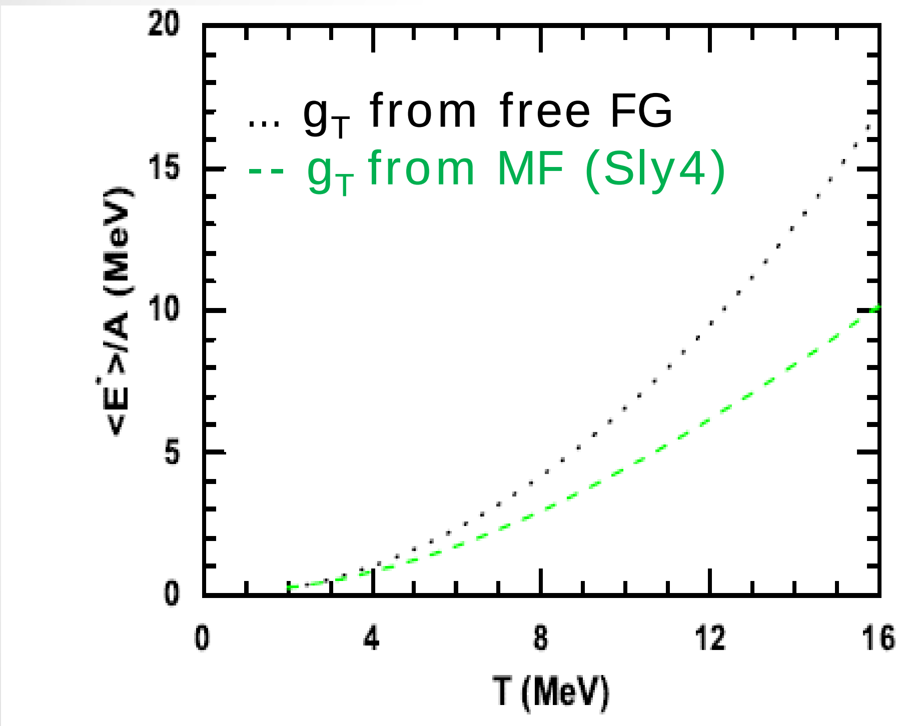
- A thermodynamically consistent formalism to calculate matter composition from a given microscopic energy functional

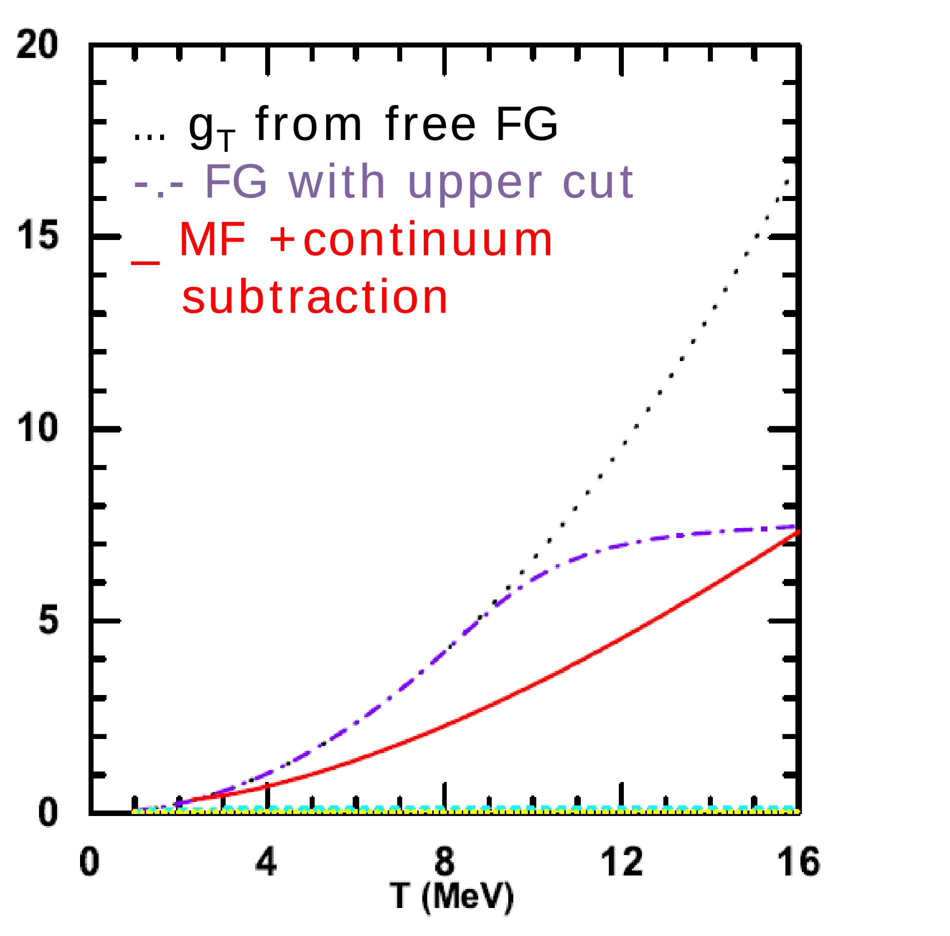
=> First microscopic evaluation of the impurity factor

- Important differences wrt Saha equation
  - Subtraction of continuum states: reduced partition sum
  - In-medium modified surface energies
  - Rearrangement terms modify even the average quantities
- Important differences wrt calculations in the WS cell
  - Center of mass motion favours the appearence of light clusters
  - Bimodal cluster distributions => increase of Qimp!
  - Cluster melting => Z=2 dominance close to the core at high temperature

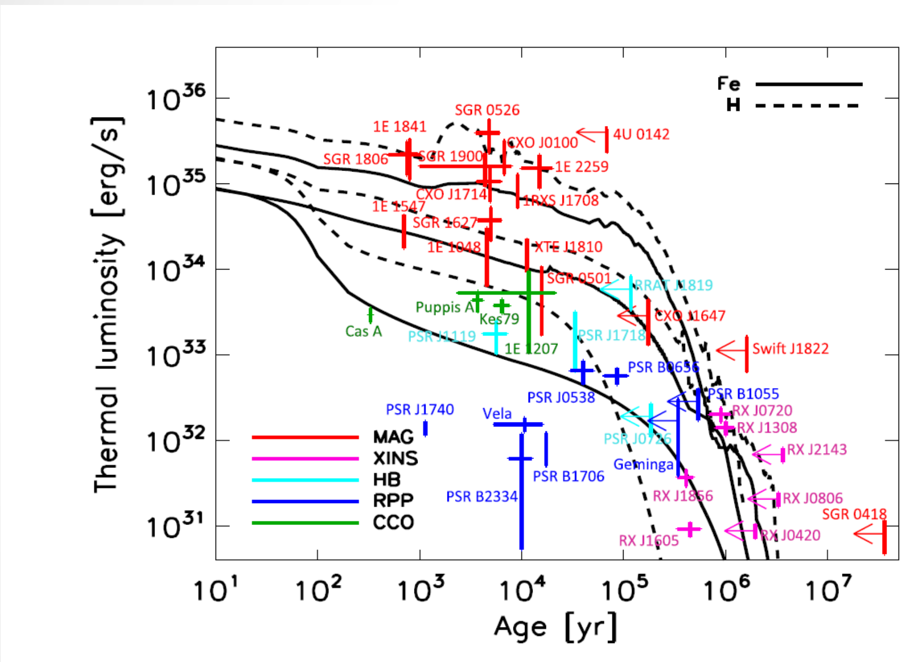
- Pasta contribution?

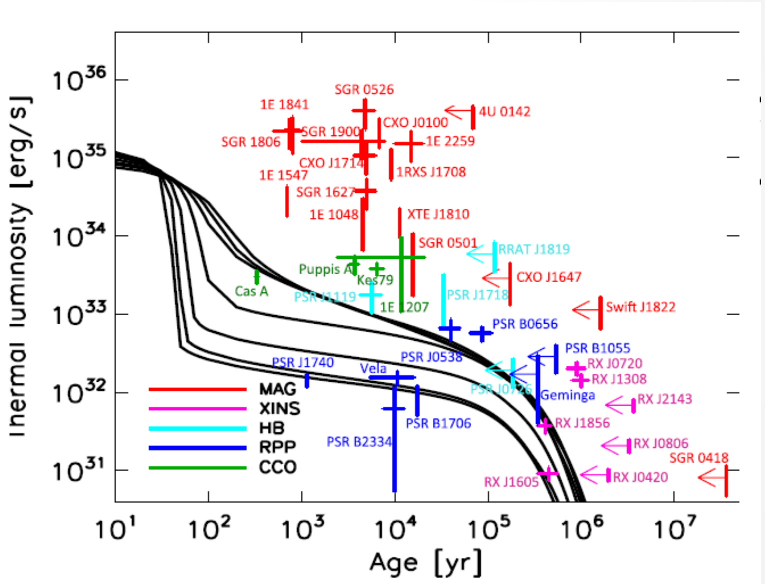
Effect of the microscopic entropy and continuum subtraction



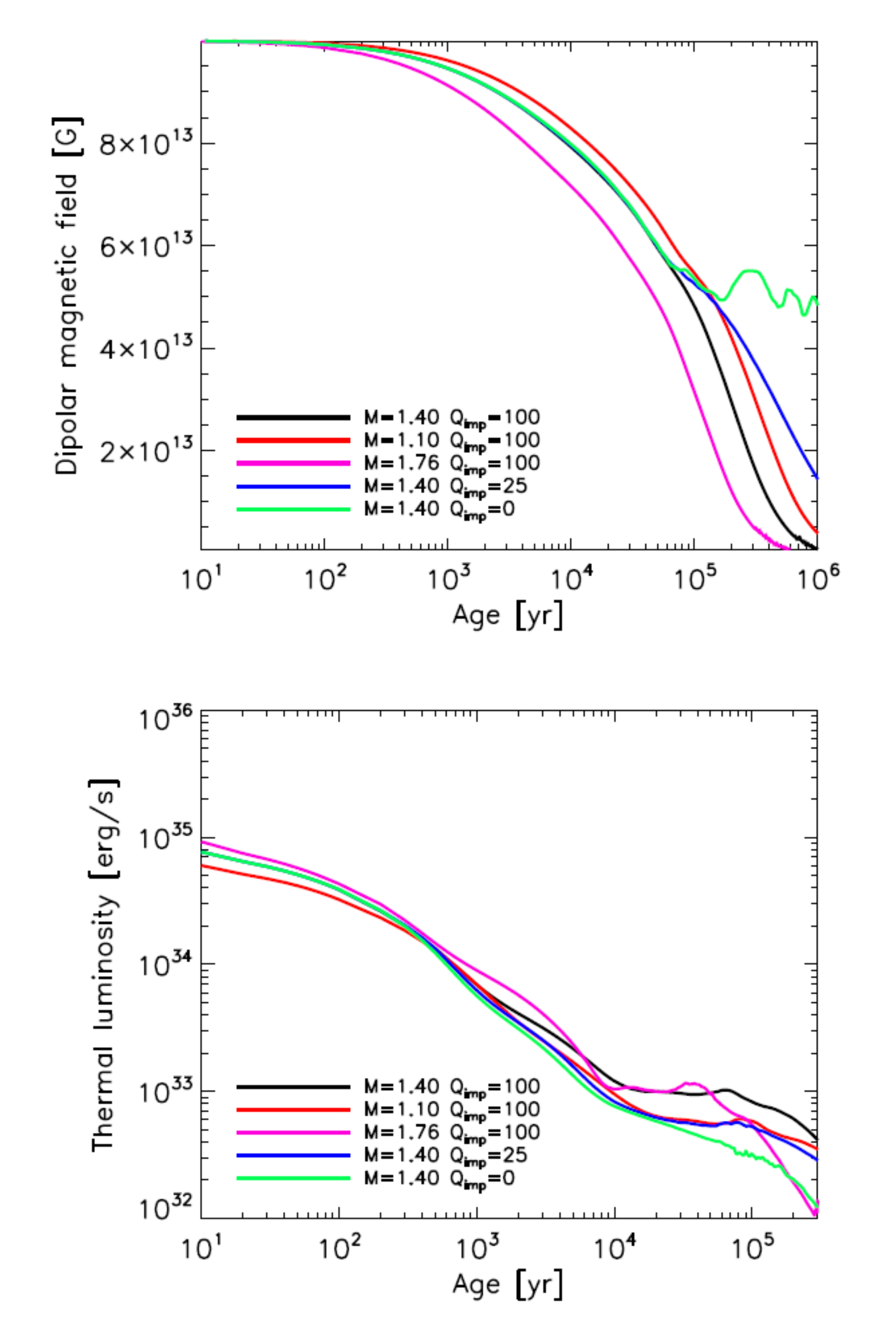


S.Mallik, FG, PRC 2021



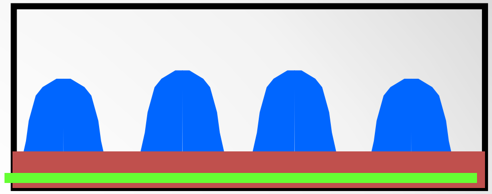


D.Vigano et al, MNRAS 434(2013)123



D.Vigano et al, MNRAS 434(2013)123

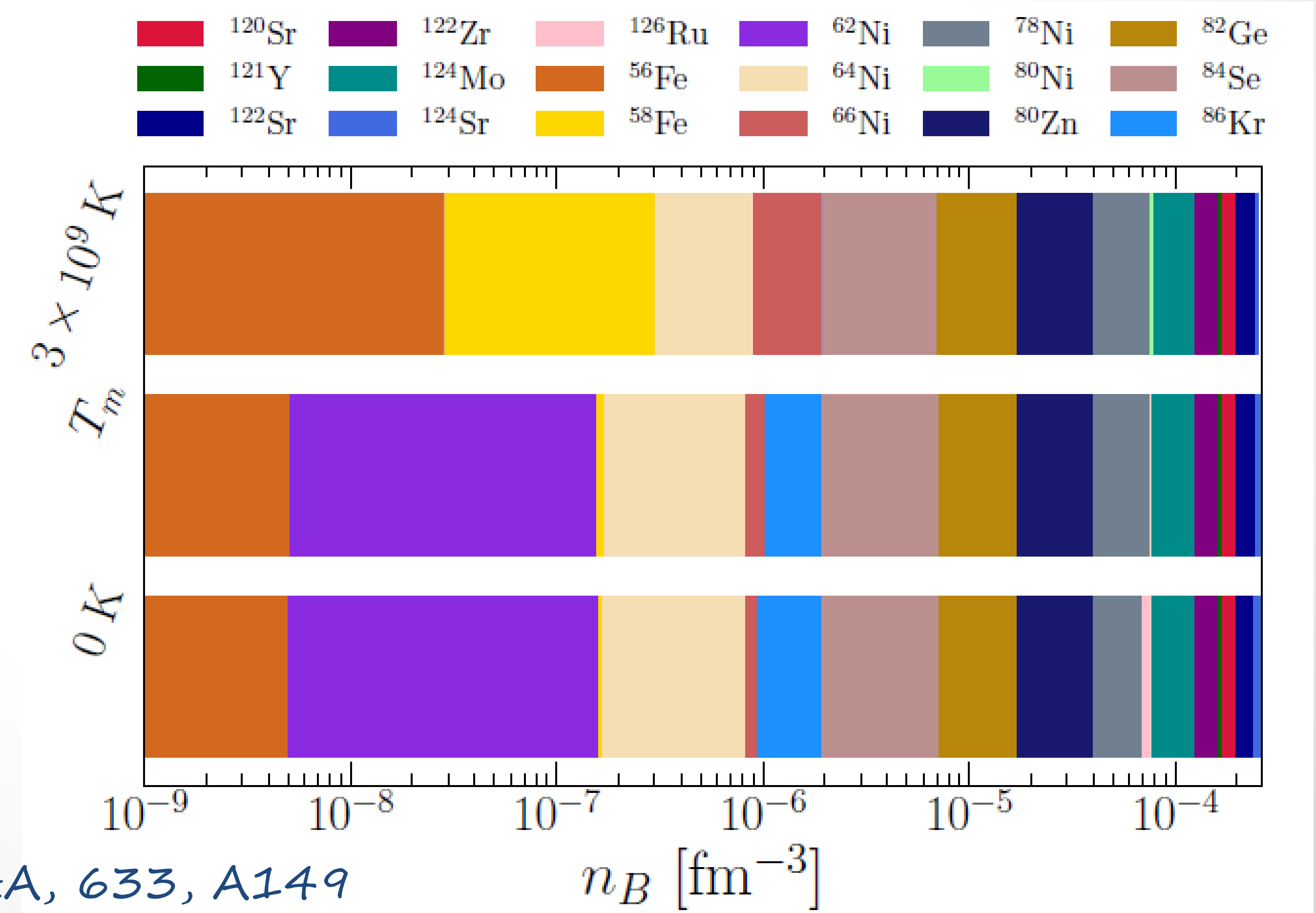
OCP with cluster DoF



$$\mathcal{F}^{OCP}(A,Z,\rho_{gq}) = \mathcal{F}(\rho_{gq}) + \frac{F_{AZ}}{V_{WS}} = \mathcal{F}_{WS}$$

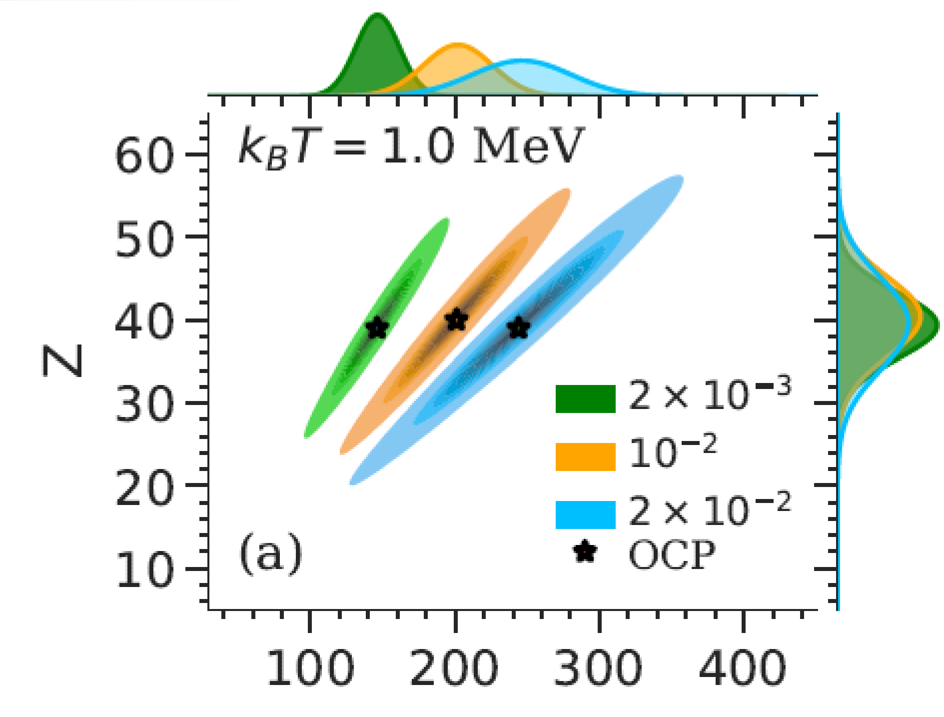
- Below drip: F_{AZ} is just the HFB free energy

BSK-24

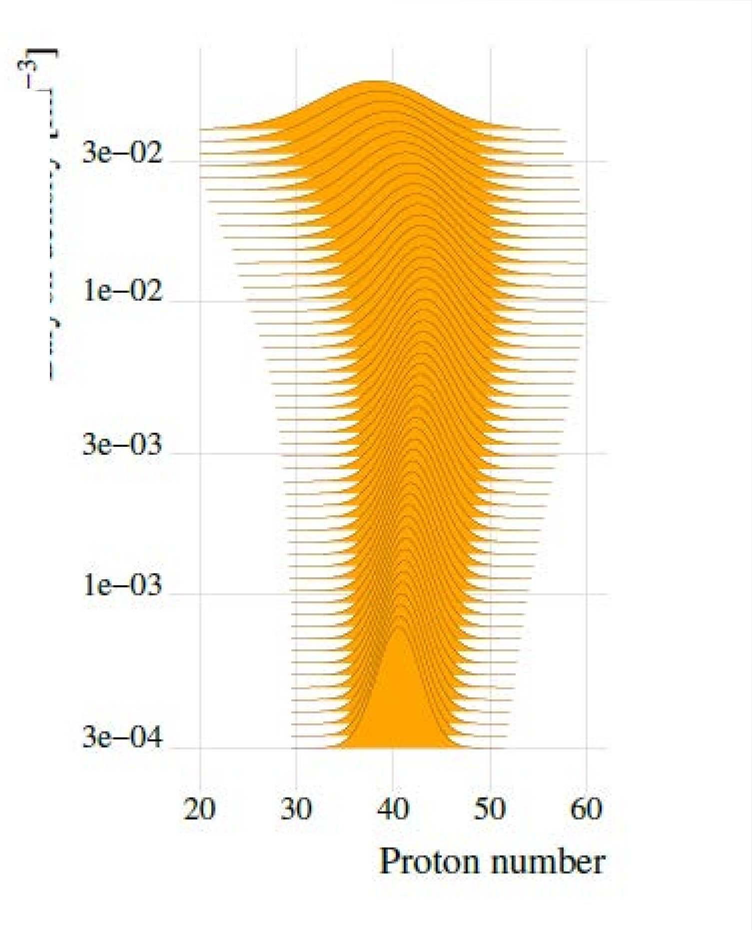


Fantina 2020, A&A, 633, A149

Nuclear distribution in the inner crust



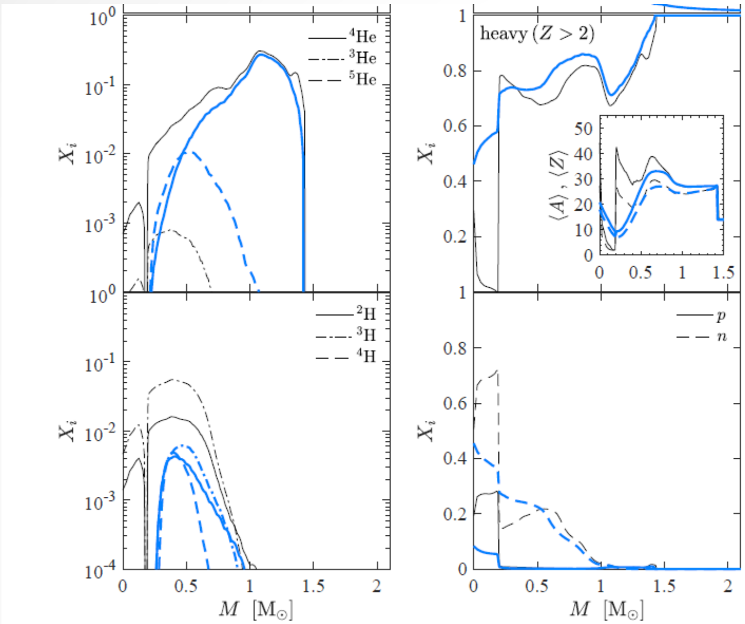
Dinh-Thi 2022, to be submitted



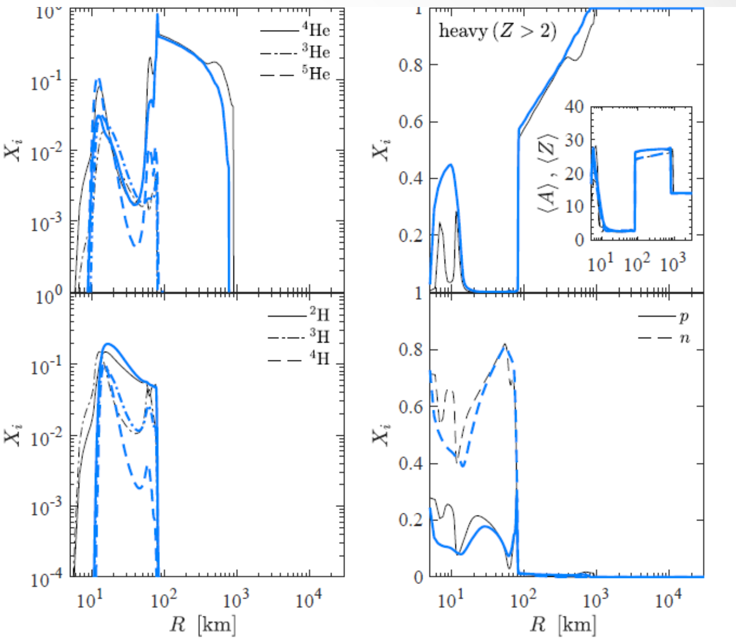
Carreau 2020, A&A, 640, A77

T.Fischer et al Phys. Rev. C **102**(2020) 055807

SN dynamics and cluster in-medium effects

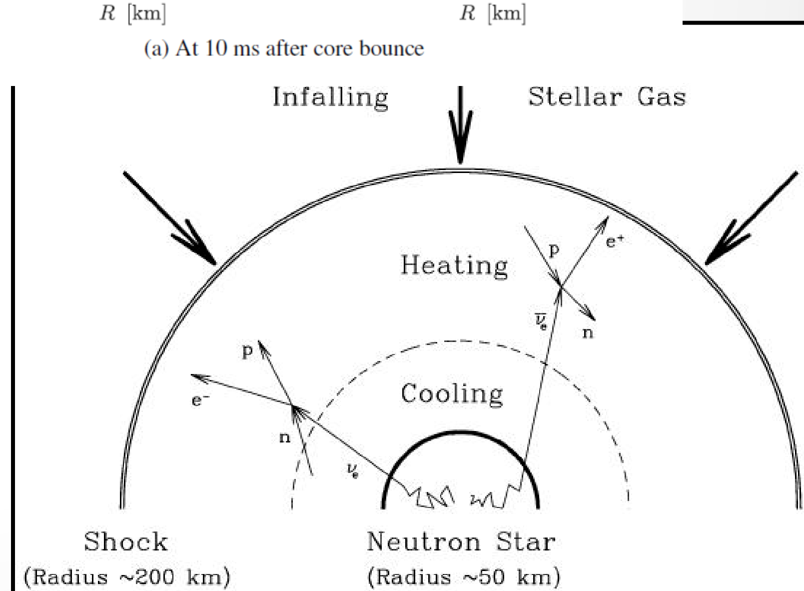


(a) At about 0.5 ms before core bounce



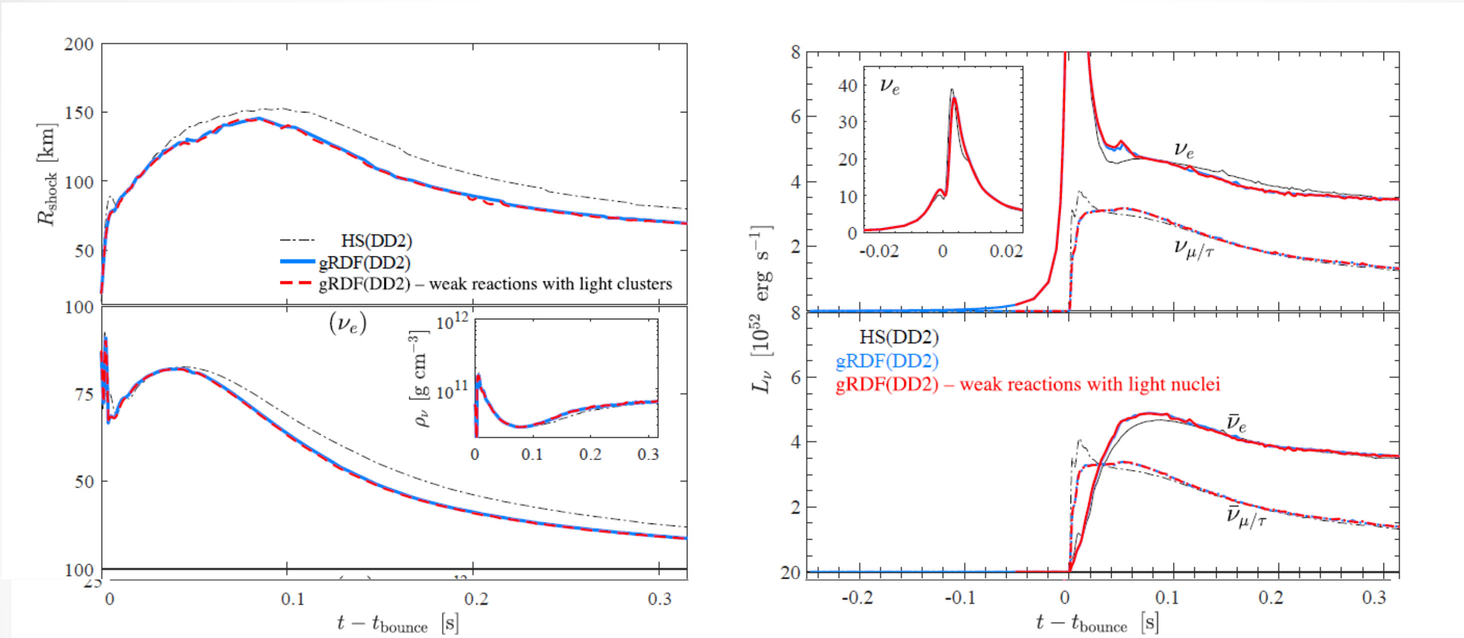
(a) At 10 ms after core bounce

- The energy deposition in the gain region depends on the position of the ν–sphere
- Coherent scattering off nuclei is a crucial source of opacity
- Composition depends on the in-medium modifications to the binding energy
-



T.Fischer et al Phys. Rev. C **102**(2020) 055807

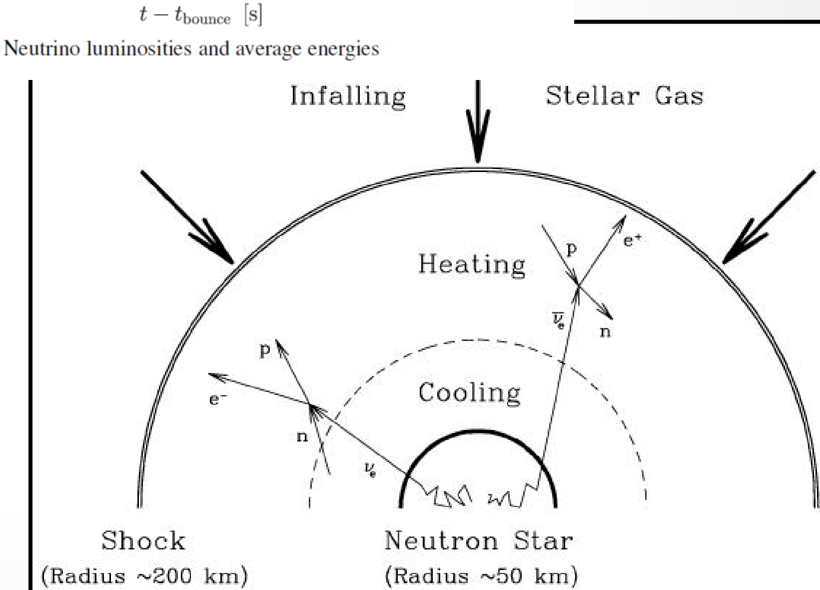
SN dynamics and cluster in-medium effects



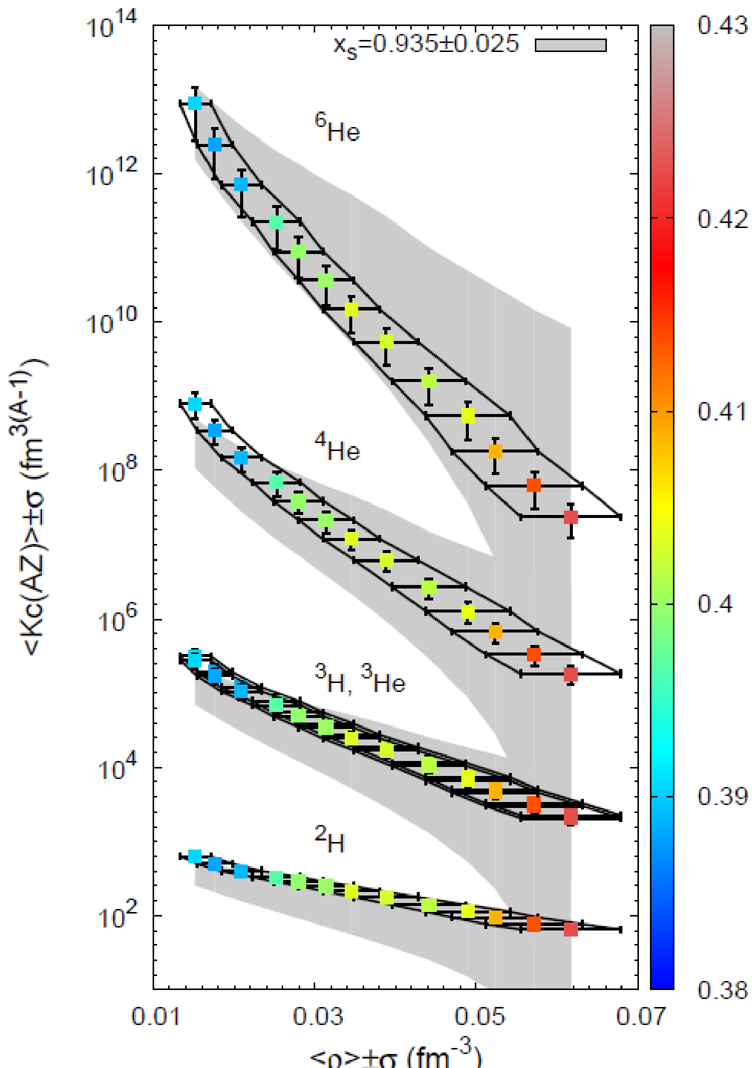
(a) Shock radii and neutrinospheres

(b) Neutrino luminosities and average energies

- The energy deposition in the gain region depends on the position of the ν–sphere
- Coherent scattering off nuclei is a crucial source of opacity
- Composition depends on the in-medium modifications to the binding energy
-

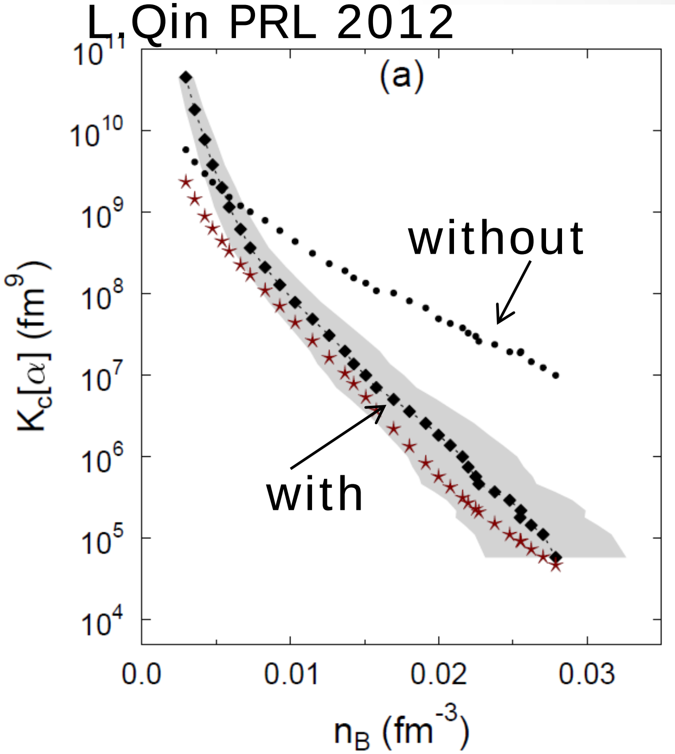


Chemical constants from multi-fragmentation



$$K_c(A,Z) = \frac{\rho_{pa}(A,Z)}{\rho_{pa}(1,1)^Z \ \rho_{pa}(1,0)^N}$$

L.Qin PRL 2012



R.Bougault & INDRA coll. JPG (2019)
H.Pais & INDRA coll. PRL (2020)

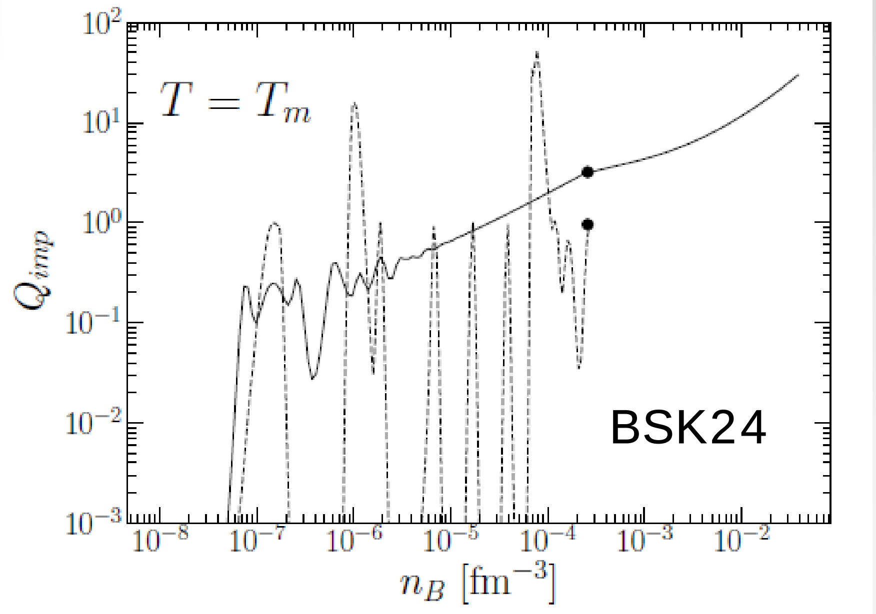
Applications

- Impurity factor

=> extension to pasta to be done

- e-transport coefficients

=> To be calculated



T.Carreau, A.Fantina, FG submitted to A&A

$$\kappa = \frac{\pi k_F^3 T}{12 e^4 m_e^{*2} \Lambda_{ep}^{\kappa}},$$

$$\sigma = \frac{k_F^3}{4\pi e^2 m_e^{*2} \Lambda_{ep}^{\sigma}},$$

$$\eta = \frac{k_F^5}{60\pi e^4 m_e^{*2} \Lambda_{ep}^{\eta}},$$

$$\Lambda_{ep}^{\kappa,\sigma}(A,Z,d) = \int_{q_0}^{2k_F} dq\, q^3 u^2(q) S_q(A,Z,d) \left(1 - \frac{q^2}{4m_e^{*2}}\right)$$

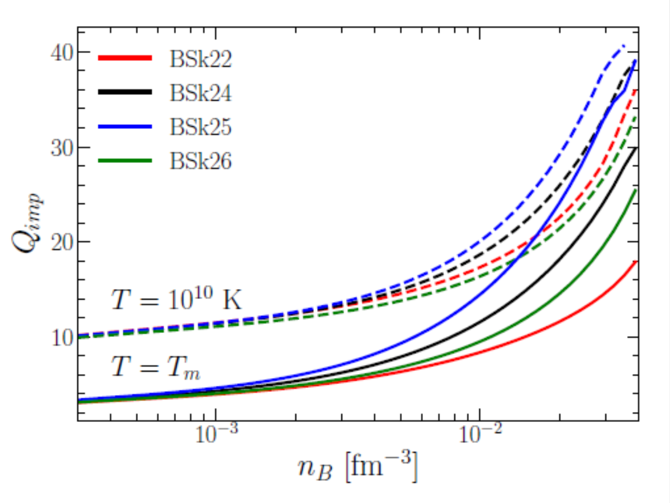
$$\Lambda_{ep}^{\eta}(A,Z,d) = \int_{q_0}^{2k_F} dq\, q^3 u^2(q) S_q(A,Z,d) \left(1 - \frac{q^2}{4m_e^{*2}}\right)\left(1 - \frac{q^2}{4k_F^2}\right)$$

$$\Lambda_{ep}^{\kappa,\sigma,\eta} = \sum_{A,Z,d} p_{AZ,d}\, \Lambda_{ep}^{\kappa,\sigma,\eta}(A,Z,d)$$

Potekhin, et al. (1999), A&A, 346, 34
Chugunov & Yakovlev (2005) ARep, 49, 724

Phenomena

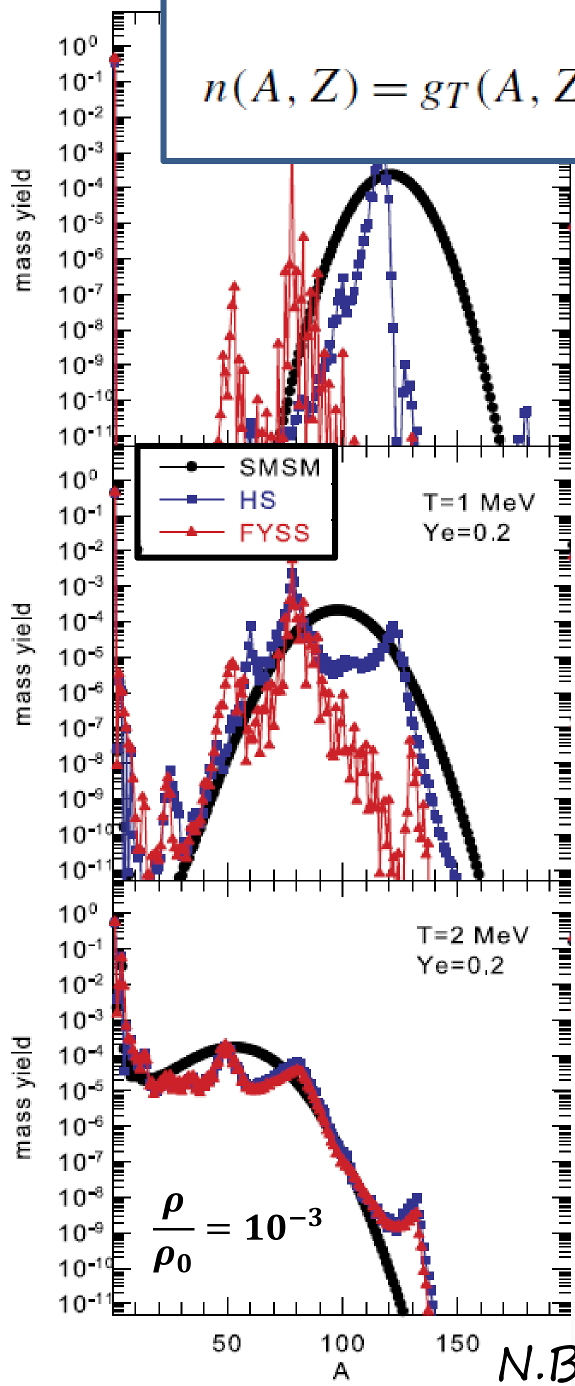
- NS oscillations
- PNS cooling (SN1987a ??)
- Mergers ???



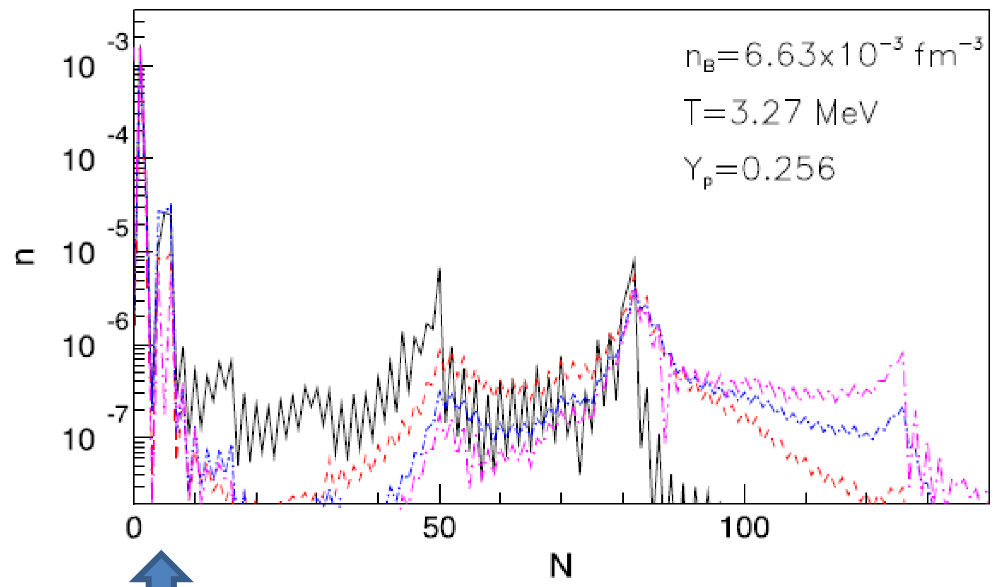
Strategy

- What exactly do we need to calculate?
- Which format (table, code..) ?
- Microscopic functional: calculate for BSK22-26 ?
- Meta-modelling: Tews functionals? Most probable posterior EoS only?

$$n(A,Z) = g_T(A,Z)\left(\frac{M_{A,Z}T}{2\pi\hbar^2}\right)^{3/2}\exp\left[\frac{(A-Z)\mu_n + Z\mu_p - M(A,Z) + \delta E}{T}\right]$$



A.Raduta, FG NPA 983(2019)252



Different level densities (g_T)

Different models (M, $\mu(\rho)$, δE, g_T)

N.Buyukcizmeci et al NPA 907(2013)13

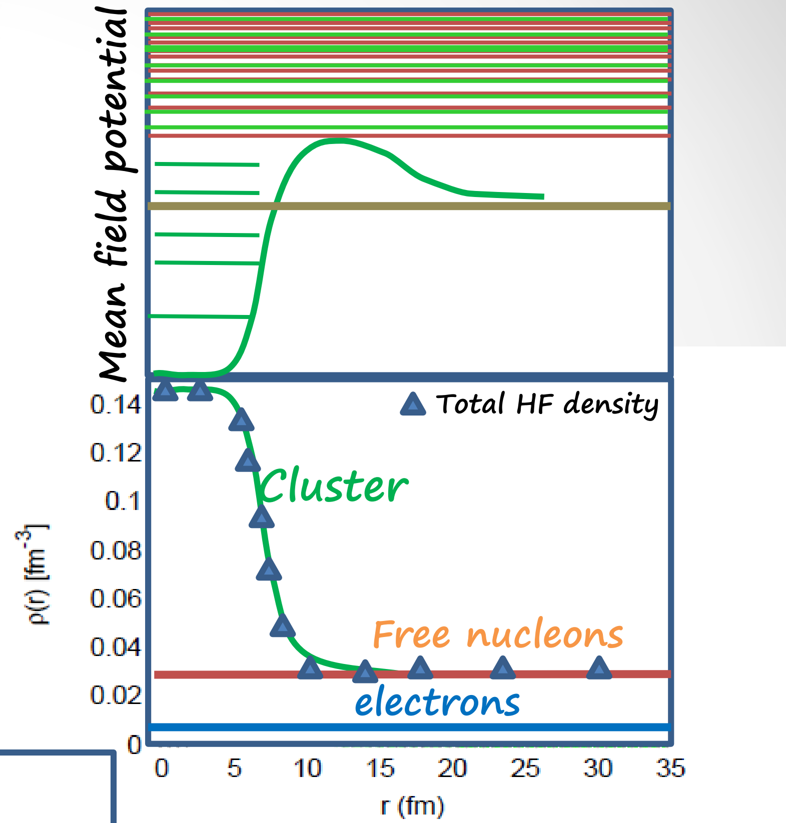
T>0: continuum states

- Double counting of continuum states if we switch to cluster DoF
- Easy subtraction in the GC ensemble

$$Z_{\beta\mu_n\mu_p} = \prod_{i,q}\left(1+\exp\left(\alpha_q - \beta e_i^q\right)\right)$$

$$\Omega_N = \Omega_{Ng} - \Omega_g \qquad \Omega_N = -T\ln \mathscr{Z}^{(N)}_{\beta\mu_n\mu_p}$$

Tubbs&Koonin, ApJ 232 (1979) L59
Bonche,Levit,Vautherin NPA427(1984)278



$$F_N\left(A, I, \rho_g, y_g\right) =$$

$$= -TV_N \ln \mathfrak{z}^{mf,N}_{\beta,\mu_n,\mu_p} + \mu_n N_n + \mu_p N_p + E_{coul} + E_{surf}(A,I)$$

$$= V_N\left[v(n_c,\delta_c) - v(n_g,\delta_g) - \sum_q \left(U_{c,q} n_{c,q} - U_{g,q} n_{g,q}\right)\right]$$

$$- \sum_{q=n,p}\left[\frac{2V_N}{3}\left\{\xi_{c,q} - \xi_{g,q}\right\} - \mu_q N_q\right]; + E_{coul} + E_{surf}(A,I)$$

S.Mallik, FG, to be submitted

Surface tension and correlations with NM properties

$I_{crust,1.4}/I_{1.4}$

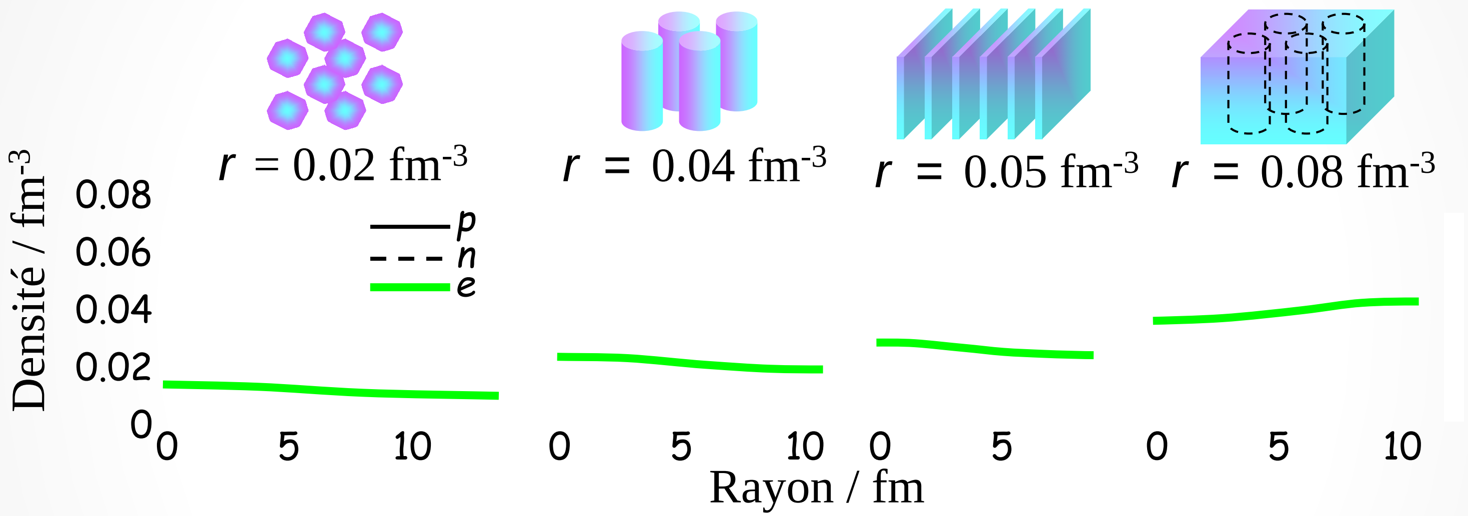
	n_{sat}	E_{sat}	K_{sat}	Q_{sat}	Z_{sat}	E_{sym}	L_{sym}	K_{sym}	Q_{sym}	Z_{sym}	m^*/m	$\Delta m^*/m$	b	p	σ_0	b_s	n_t	P_t	$I_{crust,1.4}$
LD p=3	0.01	-0.05	0.20	-0.06	-0.06	-0.24	-0.38	0.42	0.77	-0.32	0.00	0.07	-0.04	0.00	0.04	0.19	0.90	0.93	0.92
HD p=3	-0.03	0.24	0.26	-0.22	0.07	0.26	-0.08	-0.33	0.46	-0.10	-0.03	0.04	-0.10	0.00	-0.23	-0.02	0.71	0.94	0.79
LD	0.04	-0.21	0.16	-0.05	-0.04	-0.09	-0.23	0.26	0.52	-0.20	-0.01	0.04	-0.02	0.56	0.46	0.58	0.92	0.96	0.94
HD	-0.02	0.14	0.24	-0.21	0.08	0.25	-0.08	-0.31	0.42	-0.09	-0.02	0.04	-0.09	0.25	-0.09	0.18	0.73	0.95	0.79
Prior	0.02	0.12	0.21	-0.11	0.03	0.25	-0.03	-0.46	0.48	-0.11	-0.04	-0.14	-0.15	0.11	-0.08	0.10	0.40	0.96	0.72

	E_{sat}	n_{sat}	K_{sat}	Q_{sat}	Z_{sat}	E_{sym}	L_{sym}	K_{sym}	Q_{sym}	Z_{sym}	p	σ_0	b_s	σ_{0c}	β
LD+HD	-0.06	-0.05	0.33	-0.35	0.18	0.05	-0.19	-0.28	0.52	-0.14	0.13	0.06	0.12	-0.03	-0.06
LD+HD $p=3$	-0.05	-0.06	0.34	-0.35	0.18	0.03	-0.22	-0.30	0.54	-0.16	0.00	0.05	0.03	-0.02	-0.08
LD (w/ P) $p=3$	-0.00	-0.03	0.23	-0.24	0.10	-0.04	-0.33	-0.02	0.73	-0.24	0.00	0.00	0.05	0.00	-0.04
LD $p=3$	-0.07	-0.03	0.30	-0.27	0.12	0.16	-0.13	-0.35	0.50	-0.08	0.00	0.07	-0.05	0.00	-0.11
HD $p=3$	0.24	-0.03	0.29	-0.44	0.20	0.11	-0.03	-0.16	0.44	-0.15	0.00	-0.25	-0.21	0.27	-0.00
Prior $p=3$	0.19	-0.03	0.25	-0.40	0.14	0.13	-0.01	-0.25	0.42	-0.09	0.00	-0.19	-0.21	0.24	-0.05

The ambiguity is under control if we make a UNIFIED modelling

T.Carreau, PRC 2020 +
Thomas Carreau, PhD thesis

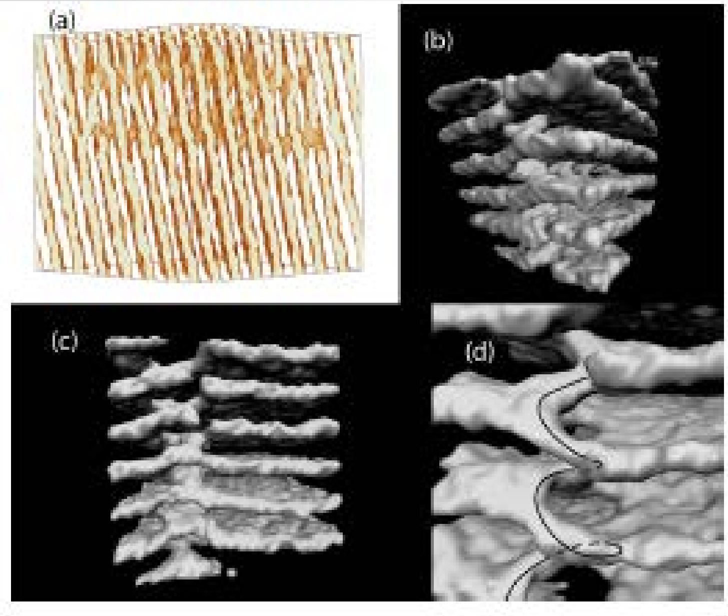
Geometry fluctuations



- $d\mathcal{F}_{MCP}(\{n_{AZ,d}\}) = 0$ leads to:

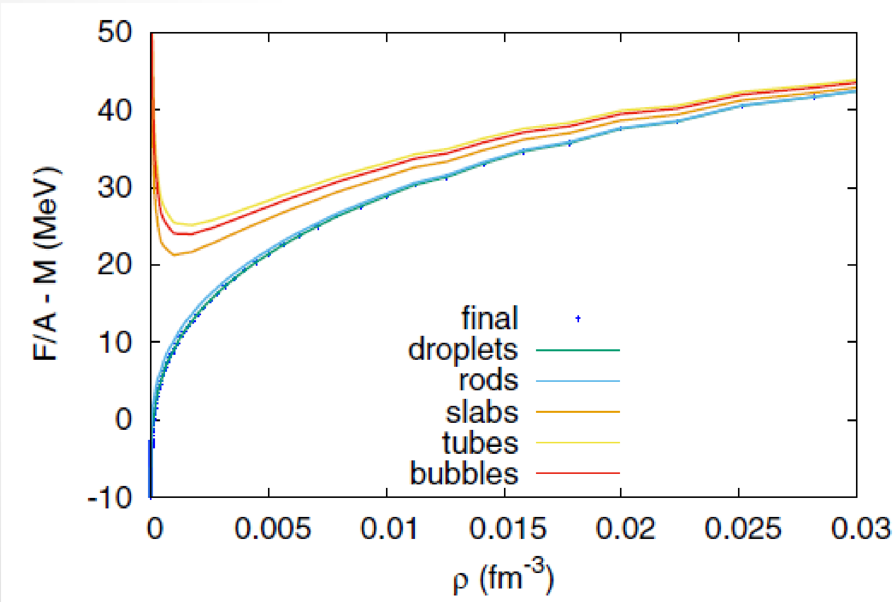
$$p_{AZ,d} \propto \exp\beta[N\mu_n + Z\mu_p - F_{i,d} + R_{AZ,d}(n_e)]$$

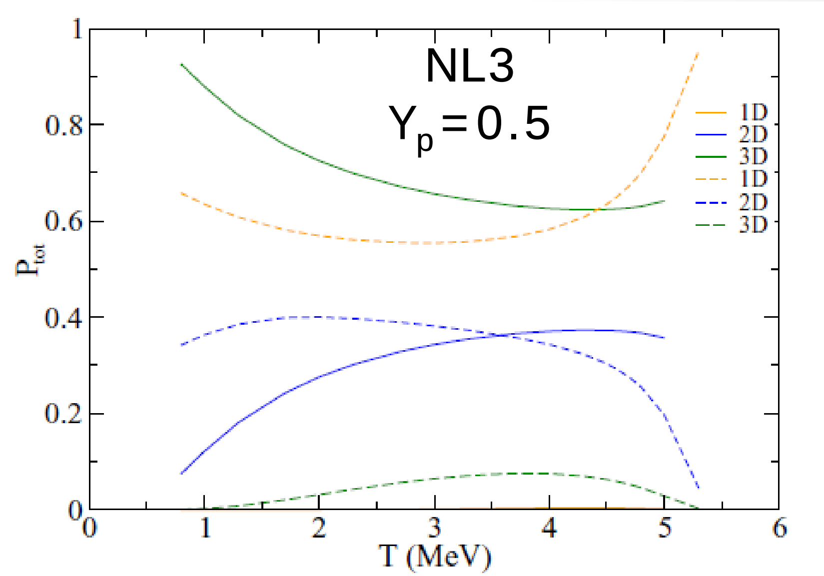
Schneider, Horowitz PRL 2015



Geometry fluctuations

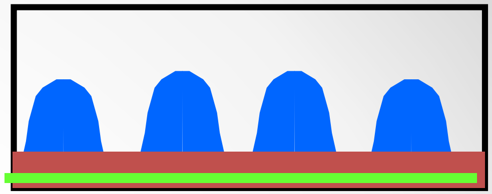
Solid: $\rho_B = 0.01$ fm^{-3}
Dashed: $\rho_B = 0.03$ fm^{-3}





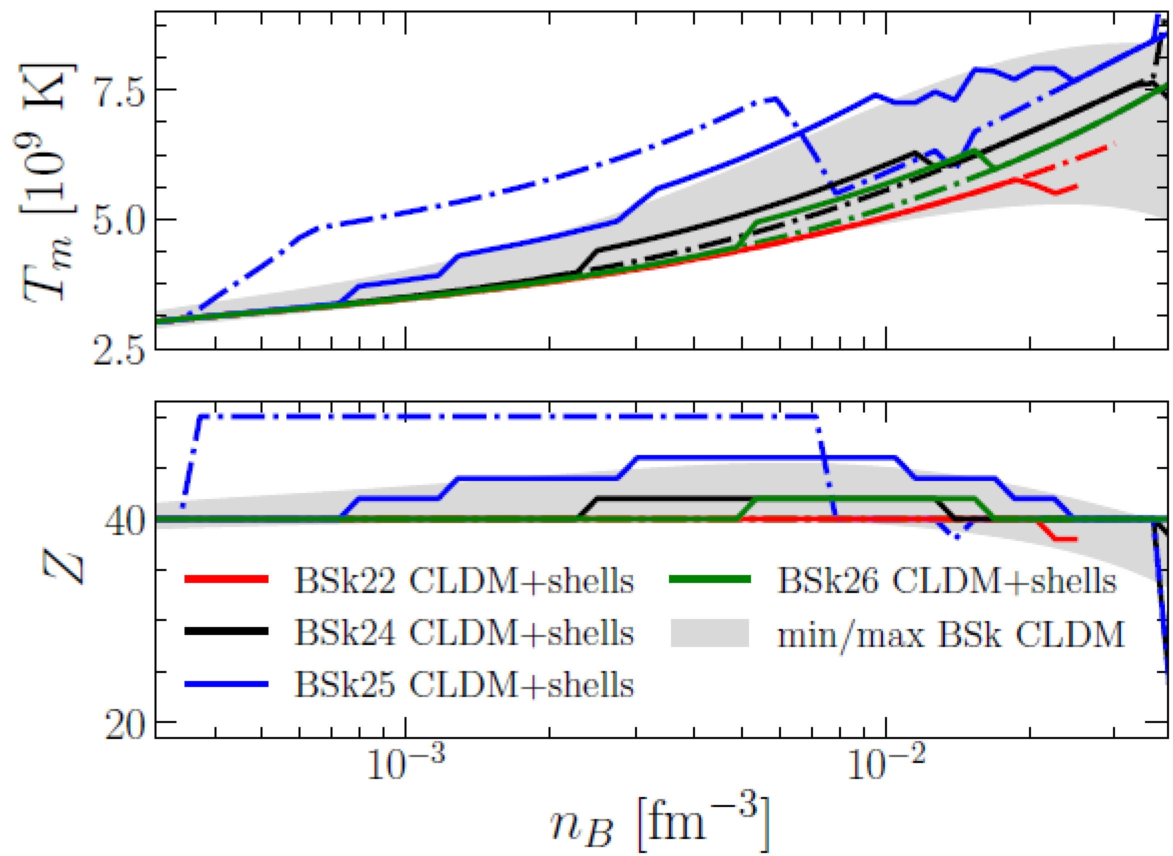
C.Barros, D.Menezes, FG, PRC 101 (2020) 035211

OCP with cluster DoF



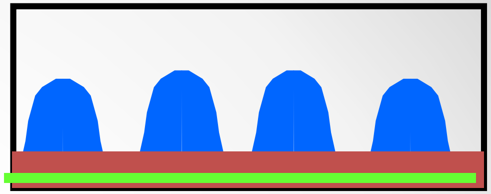
$$\mathcal{F}^{OCP}(A, Z, \rho_{gq}) = \mathcal{F}(\rho_{gq}) + \frac{F_{AZ}}{V_{WS}} = min$$

Carreau 2020, A&A, 635, A84



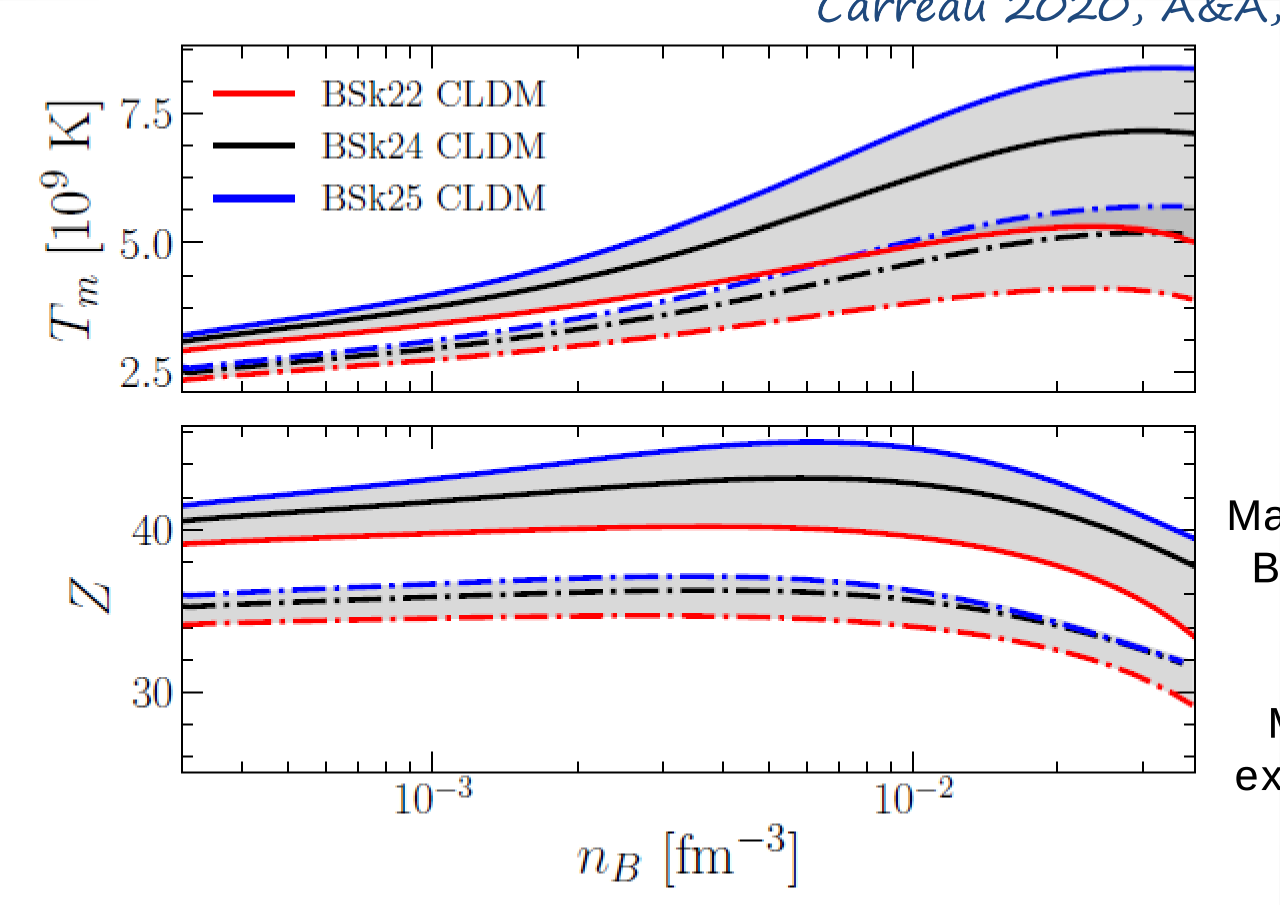
=> The uncertainty in the shell treatment is within the fonctional uncertainty.

OCP with cluster DoF



$$\mathcal{F}_{AZ}(A, Z, \rho_{gq}) = \mathcal{F}_{\mu}(\rho_{gq}) + \frac{F_i}{V_{AZ}} = min$$

Carreau 2020, A&A, 635, A84



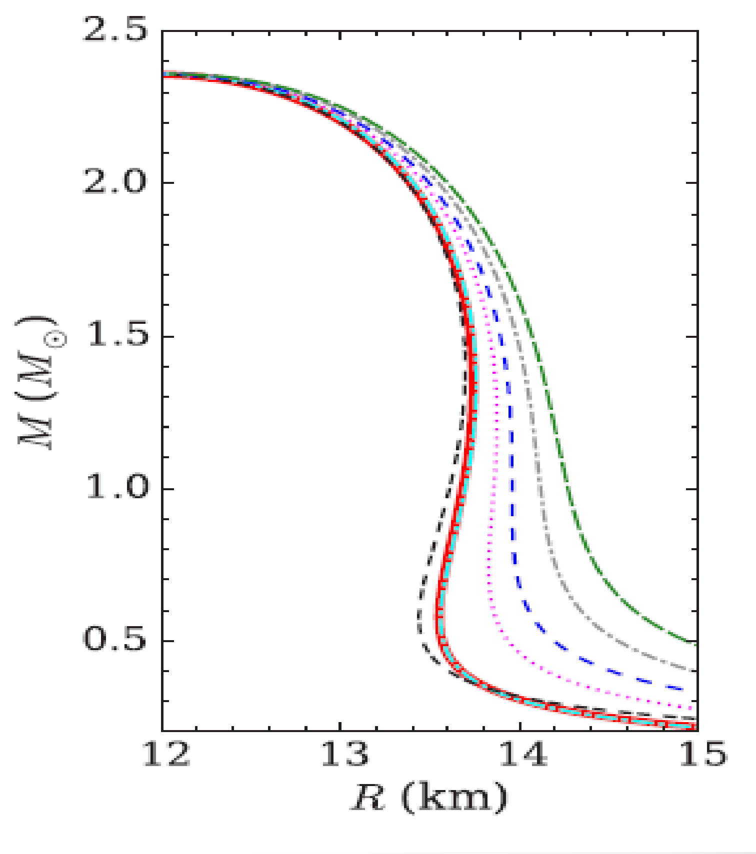
Mass fit on BSK ETF

Mass fit on exp.spherical nuclei

=> Importance of a unified treatment

Plan

1. ***Motivation: transport properties in compact stars***
2. ***From a microscopic EDF to the finite temperature nuclear distribution: unified T>0 EoS for astrophysics***
3. ***Results: melting temperature and impurity factor: the unexpected role of light nuclear clusters***



M.Fortin et al. PRC 94, 035804