Clustering and two-body correlations within extended density functional approaches

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MOdeling Nuclear STructure and REactions

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INFN - Laboratori Nazionali del Sud

Outline of the presentation

1. **Theoretical approaches for nuclear many-body problem**
   - Ab-initio vs phenomenological models based on energy density functionals (EDF)
   - Effective interaction and nuclear matter (NM) Equation of State (EoS)

2. **Extended EDF-based models: recent developments and results**
   - **Bridging ab-initio with phenomenological EDF approaches**
     - Benchmark on microscopic pseudo-data for low-density neutron matter
     - Power counting analysis based on many-body perturbative expansion
   - **Beyond mean-field: many-body correlations and clustering phenomena**
     - Neutron star (NS) crust modelization for a global and unified EoS
     - Embedding short-range correlations within relativistic approaches

3. **Further developments and outlooks**
   - Covariant formulation of the two-body quantal problem for bound states
   - Inclusion of light-clusters within non-relativistic transport theories

4. **Summary and perspectives**

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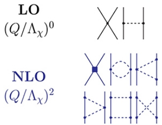
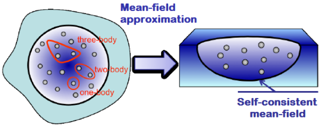
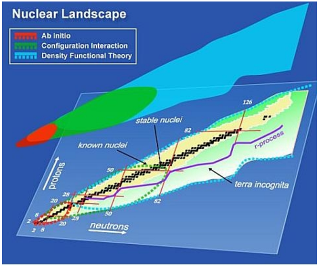
Theoretical models for EoS and finite nuclei

- **Ab-initio** approaches based on **many-body** (MB) expansion
  - Realistic or **effective field theory** (EFT) interactions
    $\Rightarrow$ Diagrammatic hierarchy (**power counting**)







- **Phenomenological** models with **effective** interaction
  - **Self-consistent** mean-field (**MF**) approximation
  - Fit of **parameters** to reproduce various **data**

- Energy Density Functional (**EDF**) theory

$$E = \langle\Psi|\,\hat{\mathcal{H}}_{\text{eff}}(\rho)\,|\Psi\rangle = \int \mathcal{E}(\mathbf{r})d\mathbf{r} \xrightarrow[\text{eq.}]{} \text{EoS}$$

$|\Psi\rangle \equiv$ independent many-particle state

  - **Isovector** component of EoS $\left(\beta \equiv \frac{\rho_n-\rho_p}{\rho}\right)$
    $\Rightarrow$ **symmetry energy** $S(\rho)$ out **saturation** ρ_0

$$\frac{E}{A}(\rho,\beta) \approx \frac{E}{A}(\rho,0)+S(\rho)\beta^2 \quad S(\rho) = \text{J}+\text{L}\left(\frac{\rho-\rho_0}{3\rho_0}\right)+\dots$$

  - Description of **ground state** and **excitations**

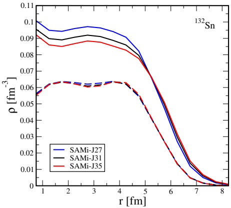
Nuclear structure: neutron skin and pygmy resonance

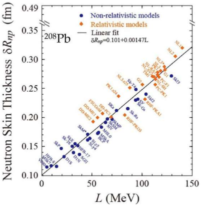
- Non-relativistic **Skyrme-like** EDF
- Structure of **neutron-rich** nuclei

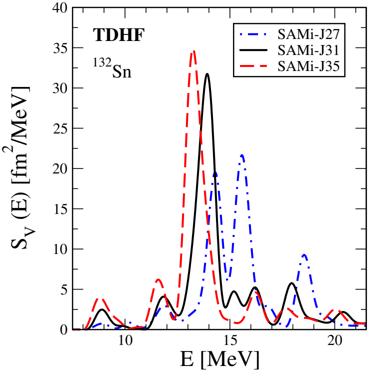
  [Zheng et al., PRC 94(1), 014313 (2016)]

  [S. Burrello et al., PRC 99(5), 054314 (2019)]

  - Neutron **skin** thickness $\Delta r_{np} \Leftrightarrow L$



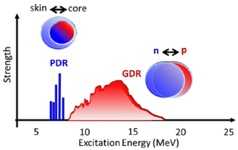


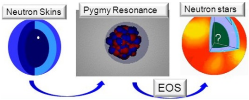


- Time-Dependent-Hartree-Fock **(TDHF)**

$$i\hbar\dot{\hat{\rho}}(t) + \left[\hat{\rho}, \hat{\mathcal{H}}_{eff}[\rho]\right] = 0$$

- **Isovector dipole** (collective) excitations:
  - **Pygmy** Dipole Resonance (**PDR**)





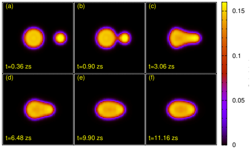
Merging nuclear structure and reaction studies

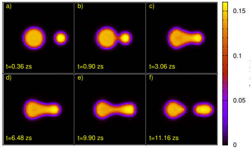
- **Pre-equilibrium** in **charge-asymmetric reactions**

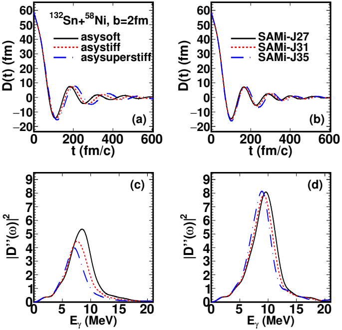
  [H. Zheng, S. Burrello, M. Colonna, V. Baran, PLB 769 (2017)]

- Interplay between **fusion** and **quasi-fission** processes
  $\Rightarrow$ formation of **super-heavy elements**

[H. Zheng, S. Burrello, M. Colonna, D. Lacroix, G. Scamps, PRC 98 (2018)]







- Same **framework** as for nuclear **structure** $\Rightarrow$ Merging with **reaction** studies
- Role of **different terms** of effective **interaction** (and EoS) on **final outcomes**
  - Importance of **momentum** dependent + **surface** terms (+ **symmetry** energy)
- Heavy ion collisions are reliable **tools** to extract **information** of EoS!

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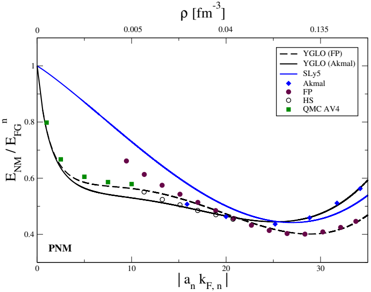
Pure neutron matter (PNM) low-density expansion

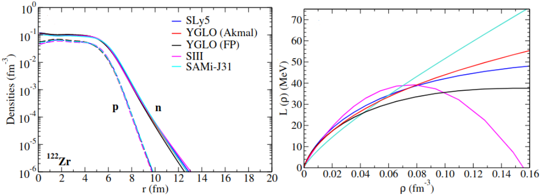
- **Dilute** PNM (a_s = -18.9 fm) ⇒ close to **unitary** limit of interacting **Fermi** gas
- **Lee-Yang** expansion in $(a_s k_F)$ from **EFT** ($\nu_i = 2, 4$ for PNM, symmetric NM)

$$\frac{E}{N} = \frac{\hbar^2 k_F^2}{2m}\left[\frac{3}{5} + (\nu_i - 1)\frac{2}{3\pi}(k_F a_s) + (\nu_i - 1)\frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a_s)^2 + \ldots\right]$$

- New **class** of **EDFs** inspired by EFT ✓ **Application** to drops & nuclei ⇒ **surface**

[S. Burrello et al., PRC 103(6), 064317 (2021)]





✗ Improving neutron **effective mass** prediction

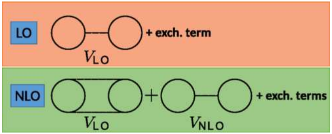
✗ Implementation in **dynamical** models

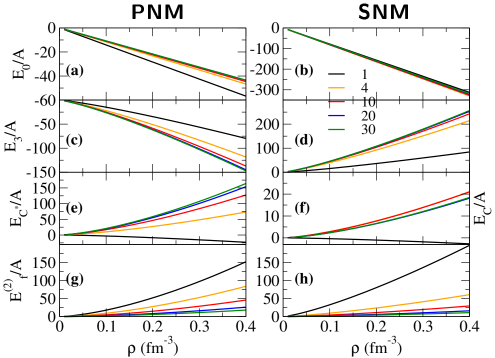
✓ Finite **temperature** (T) ⇒ ✗ compact star **modelization** (“**pasta**” formation)

[S. Burrello & M. Grasso, EPJA 58(2), 22 (2022)]

Beyond MF: towards a power counting in EDF

- Beyond MF (BMF) ⇒ **correlations** taken into account (**double-counting**)
  - **Hierarchy** of interaction (and EoS) contributions ⇒ **power counting** in EDF
- **EoSs** at next-to-leading order (**NLO**) for symmetric NM (SNM) and PNM





- (t_0, t_3) Skyrme-like V_{LO}
- **Renormalizability** analysis
  - ✓ perturbative scheme
- **Next-to-NLO** (EFT-analysis):
  - ✗ Expansion parameter
  - ✗ Breakdown scale

[S. Burrello, C.J. Yang, M. Grasso, PLB 811, 13593 (2020)]

✓ BMF study of **closed-shell** nuclei [C.J. Yang et al., PRC 106 (1), L011305 (2022)]

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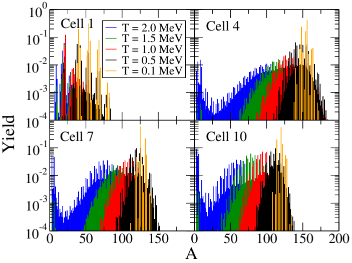
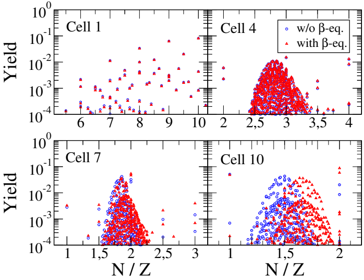
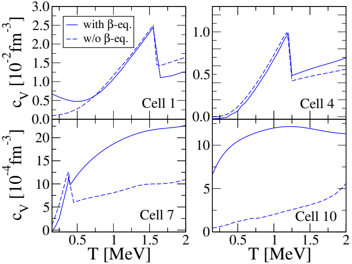
Clustering phenomena and neutron star crust

- Many-body (**short-range**) correlations below ρ_0
  - Formation of **bound** state of nucleons (**clustering**)
- **Phenomenological** models with **clusters**
  - **Dilute** matter as a **mixture** of nucleons and nuclei
    $\Rightarrow$ Nuclear statistical equilibrium (**NSE**) model
    [A. R. Raduta, F. Gulminelli, PRC 82, 065801 (2010)]
  - **Unified** description of NS EoS & **crust-core** transition
    ✓ **Composition** and **heat capacity** of NS inner crust
    [S. Burrello et al., PRC 92, 055804 (2015)]



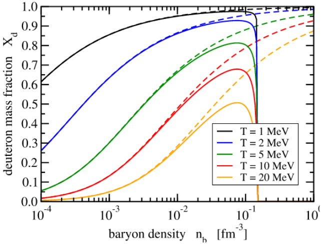




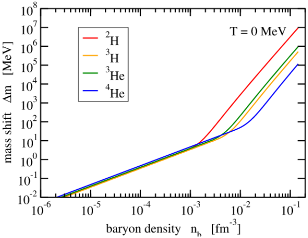
In-medium effects and cluster dissolution

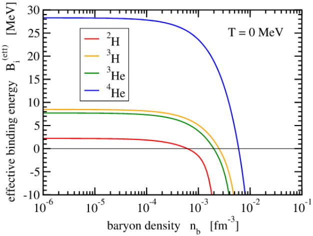
- Cluster **dissolution** approaching saturation from below
  $\Rightarrow$ **Mott effect** ruled by Pauli blocking
  - Geometrical **excluded-volume** mechanism
  - **Microscopic** in-medium effects $\Rightarrow$ **Mass-shift** (Δm)
- Generalized relativistic density functional (**GRDF**)
  $\Rightarrow$ Meson exchange with **density dependent** couplings

  [S. Typel et al., PRC 81, 015803 (2010)]



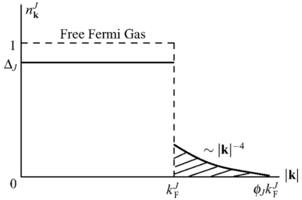
- $\Delta m^{(\mathrm{low})}$ from **in-medium** MB **Schrödinger equation** $\rightarrow \Delta m(\rho, \beta, T)$
  - **Modification** of the (effective) **binding energy** B $\rightarrow B^{\mathrm{eff}} = B - \Delta m$
- **Heuristic** extrapolation beyond **Mott density** to prevent the clusters to reappear





Mean-field framework and short-range correlations

- Cluster-free NM above n_0: Free Fermi gas (**FFG**)
  $\Rightarrow$ **step function** in momentum distribution at zero T
- Nucleon knock-out in **inelastic electron scattering**
  [O. Hen et al. (CLAS Coll.), Science 346, 614 (2014)]
  - **Smearing** of Fermi surface in cold nucleonic matter
  - High momentum tail (**HMT**) decreasing with $\sim |\mathbf{k}|^{-4}$



- Nucleon-nucleon short-range correlations (**SRCs**)
  - **Tensor** components or **repulsive** core of nuclear forces
  - **Two-body** (2B) correlations in np $^3S_1$ channel $\Rightarrow$ **quasi-deuteron**
  - Pairs amount to $\approx 20\%$ of the nucleon density
- Embedding SRCs in **GRDF** model through **in-medium modifications** of $\Delta m_i^{(\mathrm{high})}$

Quasi-deuterons as surrogate for SRCs in GRDF

- $T = 0 \Rightarrow$ **boson condensate** of deuterons under chemical potentials **equilibrium**
  - With **scalar** (S_i), **vector** (V_i) and **rearrangement** $(W_i,\ W_i^{(r)})$ potentials $(i = nuc, d)$

$$\mu_d = \mu_n + \mu_p \Rightarrow \quad \boxed{m_d^* + \Delta m_d^{(\mathrm{high})} + V_d' = \sqrt{k_n^2 + (m_n^*)^2} + V_n' + \sqrt{k_p^2 + (m_p^*)^2} + V_p'}$$

$$m_i^* = m_i - S_i \qquad S_i = \chi_i A_i C_\sigma n_\sigma \qquad V_i = \chi_i A_i \left(C_\omega n_\omega + C_\rho n_\rho\right)$$

$$W_i = \frac{1}{2}\left(C_\omega' n_\omega^2 + C_\rho' n_\rho^2 - C_\sigma' n_\sigma^2\right) \qquad V_i' = V_i + W_i + W_i^{(r)}$$

$$W_i^{(r)} = n_d \frac{\partial \Delta m_d^{(\mathrm{high})}}{\partial n_i} \qquad C_j = \frac{\Gamma_j^2(n_b)}{m_j^2} \qquad C_j' = \frac{dC_j}{dn_b}, \qquad j = \sigma, \omega, \rho$$

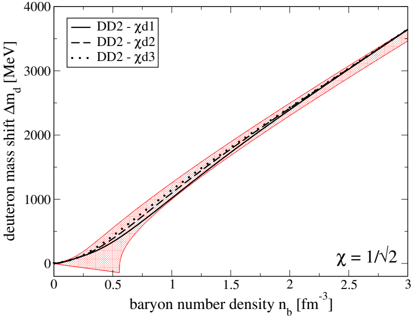
- $m^*_{\mathrm{nuc}} \geq 0 \Rightarrow 0 \leq X_d \leq \min\left\{X_d^{(\mathrm{max})}, 1 - |\beta|\right\},\ X_d^{(\mathrm{max})} = \dfrac{m_{\mathrm{nuc}}}{\chi_d C_\sigma n_b} \xrightarrow[n_b \to \infty]{} 0$
- Crucial role of **scaling factor** $\chi_d \equiv \chi$ for the **deuteron-meson** coupling strenght
  - $\chi = 1 \Rightarrow$ **same** strength as for **free** nucleons
  - $\chi < 1 \Rightarrow$ **in-medium effects** and description of chemical **equilibrium constant**

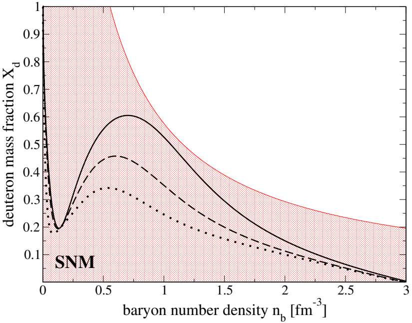
[L. Qin et al., PRL 108, 172701 (2012); R. Bougault et al., J. Phys. G 47, 025103 (2020)]

Deuteron mass-shift parametrization: $\chi = 1/\sqrt{2}$

- **Unified** mass-shift **parameterization** $(\gamma = 1)$ [S. Burrello, S. Typel, EPJA 58, 120 (2022)]

$$\Delta m_d(x) = \frac{ax}{1+bx} + cx^{\eta+1}\left[1-\tanh(x)\right] + fx^{\gamma}\tanh(gx), \qquad x = \frac{n_b}{n_0}$$





	a	b	c	η	f	g
DD2 - χd1	541.726060	243.472387	99.677247	1.656159	181.113975	0.18
DD2 - χd2	541.726060	243.472387	70.476986	1.230947	181.113975	0.22
DD2 - χd3	541.726060	243.472387	41.777908	0.257252	181.113975	0.26

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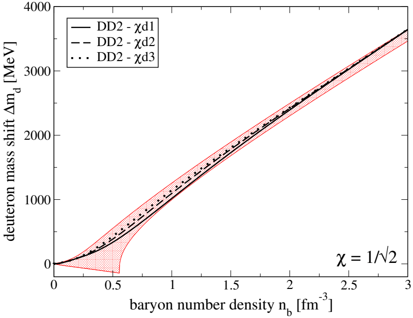

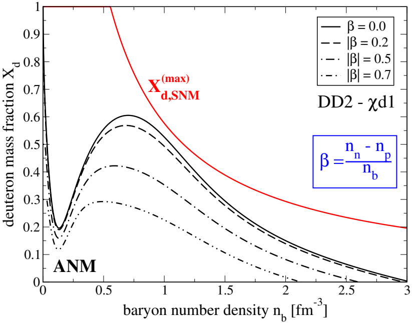

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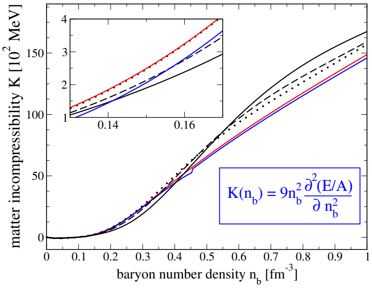
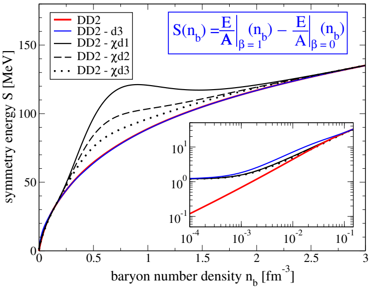
Impact on SNM EoS and symmetry energy

- **Softening** of the SNM EoS at ρ_0 and **stiffening** of symmetry energy at high-ρ

[S. Burrello, S. Typel, EPJA 58, 120 (2022)]





	DD2	DD2-d3	DD2-χd1	DD2-χd2	DD2-χd3
$K(\rho_0)$ [MeV]	242.7	199.6	185.3	207.3	240.3
L [MeV]	57.94	56.49	67.50	67.50	67.50

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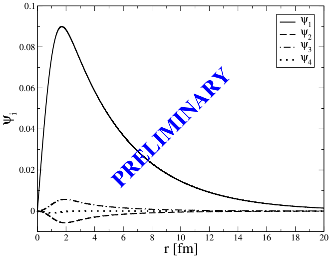
Covariant formulation of 2B quantal problem

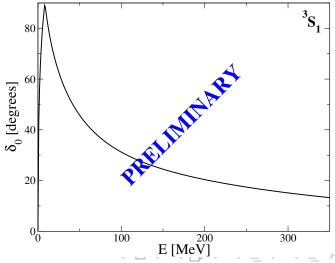
- Single-nucleon **momentum distribution** ⇒ in-medium 2B **wave function** (wf)
- **Self-consistent** calculation with **relativistic MF** effective interaction
- **Covariant** formulation of 2B **quantal** problem
  - **Bethe-Salpeter** approach (existence of negative-norm **"ghost"** states)
  - **Breit** equation (singular operators unmanageable non-perturbatively)
  - **Two-body Dirac equations** (2BDEs) of Dirac's **constrained dynamics**

    [H. W. Crater & P. Van Alstine, Annals Phys. 148 (1983) 57-94]

✓ Covariant description of deuteron **bound** and **scattering** states through 2BDEs

[S. Typel & S. Burrello, in preparation]



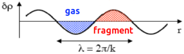


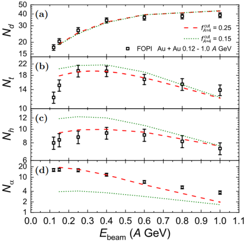
Clusters in non-relativistic transport theories

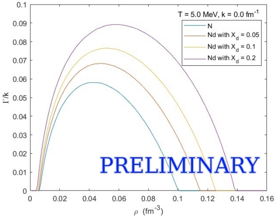
- **Kinetic** approach to production of **light nuclei** undergoing the Mott effect
  - BUU equations for **distribution functions** $f_j^{A\leq 4}$ + cut-off ($\epsilon_j \equiv$ single-particle E)

$$(\partial_t + \nabla_p \epsilon_j \cdot \nabla_r - \nabla_r \epsilon_j \cdot \nabla_p) f_j = I_{coll}[f_j] \quad \Rightarrow \quad \partial_t(\delta f_j) + \nabla_r(\delta f_j)\cdot\nabla_p \epsilon_j^0 - \nabla_p f_j^0 \cdot \nabla_r(\delta\epsilon_j) = 0$$

- Inclusion of Δm_j and P_{Mott} in collision integral I_{coll} (in progress) [see R. Wang's talk]
- Impact on spinodal instabilities (underlying **larger fragments** formation)
  - Linearized **Vlasov equations** for SNM+d under **small fluctuations** $f_j \approx f_j^0 + \delta f_j$
- Enhanced **instability growth** rate Γ/k of **density** fluctuations $\delta\rho$
  - Large effect at higher T ($X_d \neq 0$ for $(\rho, T) \lesssim (0.1\ \mathrm{fm}^{-3}, 15\ \mathrm{MeV})$)







[R. Wang et al., arXiv:2305.02988 (PRC)]

[in collaboration with M. Colonna and R. Wang]

Clusters in non-relativistic transport theories

- **Kinetic** approach to production of **light nuclei** undergoing the Mott effect
  - **BUU equations** for **distribution functions** $f_j^{A\leq 4}$ + cut-off ($\epsilon_j \equiv$ single-particle E)

$$(\partial_t + \nabla_{\rm p}\epsilon_j \cdot \nabla_{\rm r} - \nabla_{\rm r}\epsilon_j \cdot \nabla_{\rm p})\, f_j = I_{coll}[f_j] \quad \Rightarrow \quad \partial_t(\delta f_j) + \nabla_{\rm r}(\delta f_j)\cdot\nabla_{\rm p}\epsilon_j^0 - \nabla_{\rm p} f_j^0 \cdot \nabla_{\rm r}(\delta\epsilon_j) = 0$$

- Inclusion of Δm_j and $P_{\rm Mott}$ in **collision integral** I_{coll} (in progress) [see R. Wang's talk]
- Impact on **spinodal instabilities** (underlying **larger fragments** formation)
  - Linearized **Vlasov equations** for SNM+d under **small fluctuations** $f_j \approx f_j^0 + \delta f_j$
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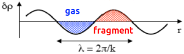
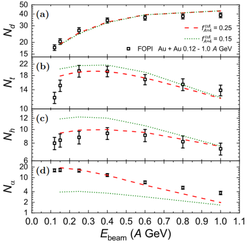
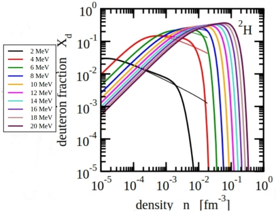
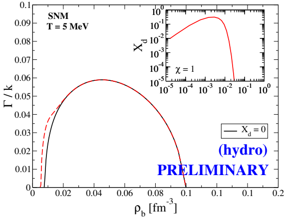


  - Large effect at **higher T** ($X_d \neq 0$ for $(\rho, T) \lesssim (0.1\ {\rm fm}^{-3}, 15\ {\rm MeV})$)



[R. Wang et al., arXiv:2305.02988 (PRC)]





[in collaboration with M. Colonna and R. Wang]

Outline of the presentation

1. **Theoretical approaches for nuclear many-body problem**
   - Ab-initio vs phenomenological models based on energy density functionals (EDF)
   - Effective interaction and nuclear matter (NM) Equation of State (EoS)
2. **Extended EDF-based models: recent developments and results**
   - Bridging ab-initio with phenomenological EDF approaches
   - Beyond mean-field: many-body correlations and clustering phenomena
3. **Further developments and outlooks**
   - Covariant formulation of the two-body quantal problem for bound states
   - Inclusion of light-clusters within non-relativistic transport theories
4. **Summary and perspectives**

Final remarks and conclusions

Main topic

- Bridging **ab-initio** with **phenomenological** EDF approaches
- Beyond **mean-field** extension: many-body **correlations** and **clustering**

Main results

- Application to **neutron drops** and **nuclei** of ab-initio-**benchmarked** EDFs
- NLO **perturbativity** of **renormalized** scheme compatible with **power counting**
- Neutron star **crust composition** and effects of clusters on **cooling process**
- Embedding **SRCs** through **quasi-deuterons** within **relativistic** approach

Further developments and outlooks

- Improving **properties** of **EFT-inspired** EDFs and full EFT-analysis
- Inclusion of SRCs at **finite T** and **light clusters** within a **kinetic approach**
- **Momentum distribution** from **in-medium wf** + comparison with **experiments**

THANK YOU FOR YOUR ATTENTION!