

Clustering and Equation of State within extended density functional approaches

1st Collaboration Meeting on
NUclear Structure, Dynamics and Astrophysics at FRIB
(NUSDAF 2025)

Physics and Astronomy Department - University of Catania (Italy)

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Authors: S. Burrello, M. Colonna, R. Wang

INFN - Laboratori Nazionali del Sud, Catania

Outline of the presentation

① Many-body (MB) correlations and clustering phenomena in nuclear systems

- Understanding Equation of State (EOS) for nuclear matter (NM)
- Phenomenological models based on energy density functionals (EDF)

② Extended EDF-based models: recent developments and results

⇒ Unified (thermodynamic) description of few-body correlations and clusters

- Embedding short-range correlations within relativistic mean-field approaches
- Global mass-shift parameterization for a multi-purposes EOS

⇒ Dynamical approach with light clusters as degrees of freedom (DOF)

- Phase-space excluded-volume approach in dilute nuclear medium
- Quasi-analytical characterization of spinodal instability and growth rates

③ Further developments and outlooks

- Connection between hydrodynamical and linearized Vlasov approach
- Extensive numerical calculations of the dynamics with light clusters
- Consistent description of fragment formation mechanisms in heavy-ion collisions

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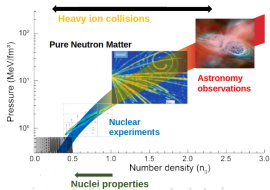
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Heavy-ion collisions: clustering effects and EOS

- Heavy-ion collisions (HIC) at $E_{\text{beam}} \approx (30 - 300) \text{ AMeV} \Rightarrow \text{EOS}$



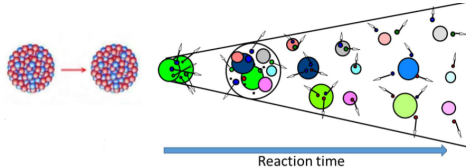
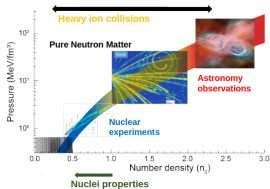
- Expansion following initial compression
 $\Rightarrow$ low density (ρ) & temperature (T)
 - Spinal instabilities $\rightarrow$
 - Few-body correlations $\rightarrow$ light clusters
- Phenomenological EDF with clusters DOF

Theoretical challenge

Consistent dynamical approach for light clusters and heavier fragments

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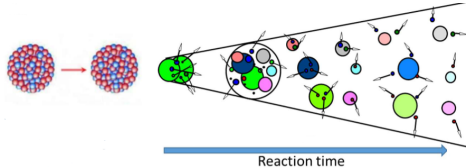
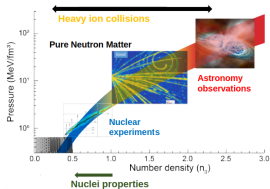
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 - From NM $\rightarrow$ clusters (nucleons+nuclei)

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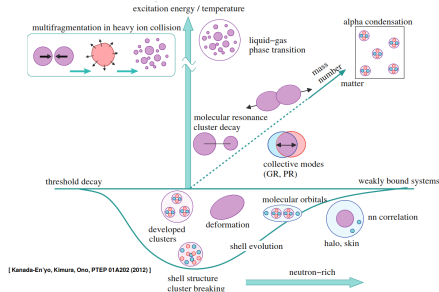
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 $\Rightarrow \text{Nucleon} \rightarrow \text{clusters (nucleons+ nuclei)}$

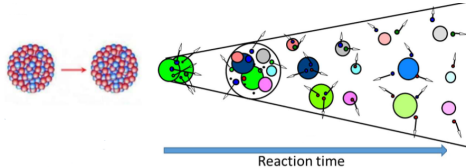
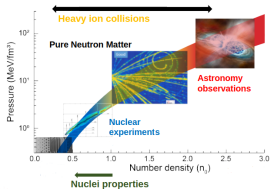
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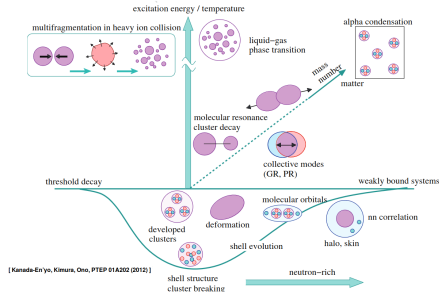


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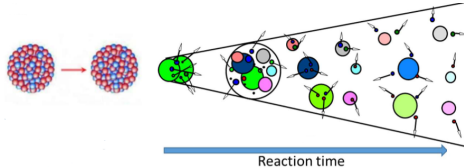
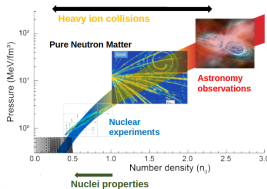


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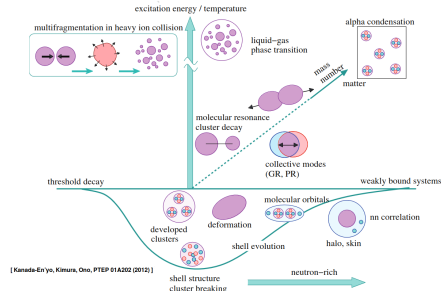
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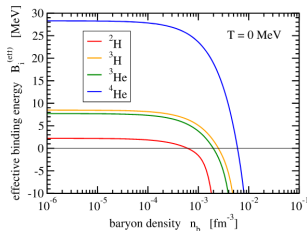
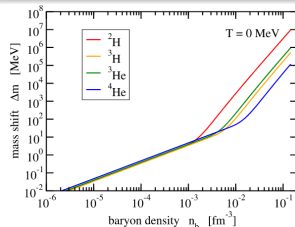


In-medium (Mott) effects and cluster dissolution

- Pauli-blocking **(Mott) effect** $\Rightarrow$ cluster **dissolution**
 - Microscopic in-medium effects
 - (Effective) **binding energy** $\rightarrow B^{\text{eff}} = B - \Delta m$
- $\Delta m^{(\text{low})}$ from in-medium Schrödinger equation (**SE**)
 - [G. Röpke, NPA 867 (2011) 66–80]
- Parameterization $\Delta m(\rho, \beta, T, P_{\text{c.m.}}) \Rightarrow$ heuristic $\Delta m^{(\text{high})}$ beyond **Mott density**
 - **Cluster dissolution** occurs when $[P_{\text{c.m.}}] > P_{\text{dissol}}$ (Mott transition)
 - **Many-body short-range correlations** (SRCs) in the continuum (see Röpke et al., Phys. Rev. Lett. 116, 052701 (2016))

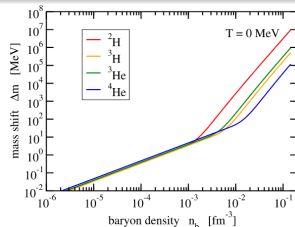
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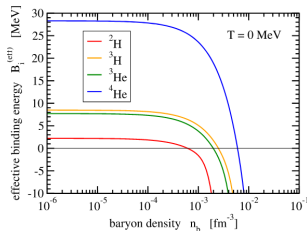


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[S. Burrello, S. Typel, EPJA 58, 120 (2022)]



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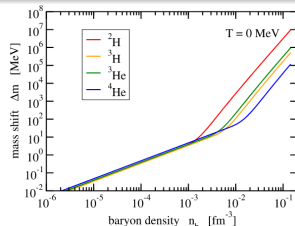
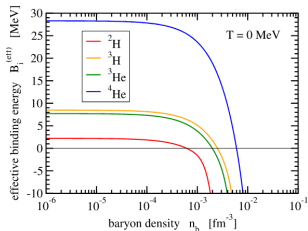
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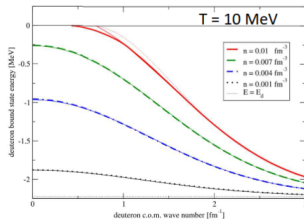
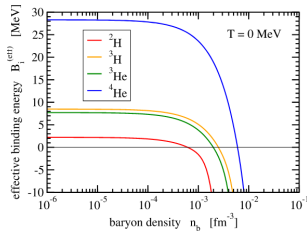
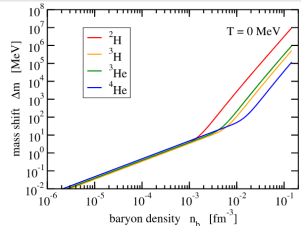
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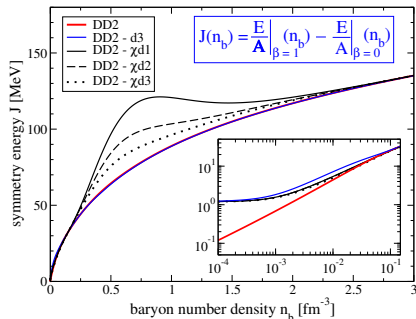
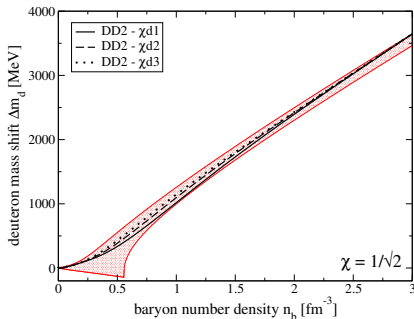
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Clusters as surrogate for SRCs in extended EDFs

- Unified mass-shift **parameterization** for bound d / np SRCs ($\rho_B \lesssim \rho_{\text{Mott}}$)

$$\Delta m_d(x) = \frac{ax}{1+bx} + cx^{\eta+1} [1 - \tanh(x)] + fx \tanh(gx), \quad x = \frac{\rho b}{\rho_0}$$



Eur. Phys. J. A (2022) 58:120
<https://doi.org/10.1140/epja/s10050-022-00765-z>

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PHYSICAL JOURNAL A



Regular Article - Theoretical Physics

Embedding short-range correlations in relativistic density functionals through quasi-deuterons

S. Burrello^{1,a}, S. Typel^{1,2,b}

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Effective phase-space excluded-volume approach

- Modeling **dynamics** of HIC at intermediate energies $\Rightarrow$ **Transport** theories
 - Boltzmann–Uehling–Uhlenbeck (**BUU**) equation for the **distribution function** f_τ

$$(\partial_t + \nabla_{\mathbf{p}} \varepsilon_\tau \cdot \nabla_{\mathbf{r}} - \nabla_{\mathbf{r}} \varepsilon_\tau \cdot \nabla_{\mathbf{p}}) f_\tau = I_\tau^{\text{coll}}[f_n, f_p, \dots], \quad \tau = n, p, d, t, h, \alpha$$

- Extended **kinetic** approaches $\Rightarrow$ Light **clusters** & **in-medium** effects
 - Solving in-medium SE $V(r, r)$ point (computationally very demanding)
 - Effective **in-medium** potentials
 - [P. Danielewicz, C. F. Barchak, NPA 533, 712 (1997)]
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$$(E)_\nu(P) \equiv \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \hat{C}_\tau^{\text{tot}}(\mathbf{p}) |\hat{\phi}_{\nu,\mathbf{p}}(\mathbf{p})|^2 \leq F_A^{\text{tot}}$$

$\hat{\phi}_{\nu,\mathbf{p}} \equiv$ free-space 1-body probability (**cluster**) distribution

$\hat{C}_\tau^{\text{tot}} \equiv$ total phase-space correlation of the medium
(including contributions from light **clusters**)

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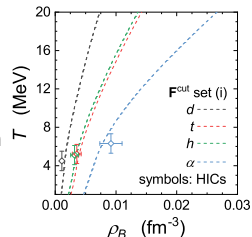
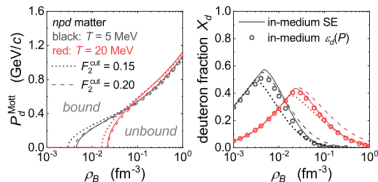
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$$\langle f_\tau \rangle_\nu(\mathbf{P}) \equiv \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} f_\tau^{\text{tot}}(\mathbf{p}) |\tilde{\phi}_{\nu, \mathbf{P}}(\mathbf{p})|^2 < F_A^{\text{cut}}$$

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arXiv > nucl-th > arXiv:2506.16437

Nuclear Theory

[Submitted on 19 Jun 2025]

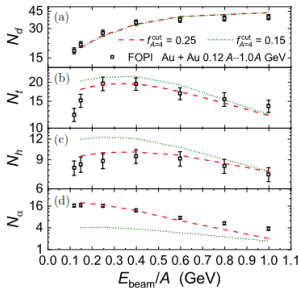
Phase-space excluded-volume approach for light clusters in nuclear medium

Rui Wang, Zhen Zhang, Stefano Burrello, Maria Colonna, Edoardo G. Lanza

Kinetic approach for HIC with light-clusters DOF

- Integrating **phase-space excluded-volume** in **transport** models $\Rightarrow$ **cut-off** in l_{τ}^{coll}
 $\Rightarrow$ **Description** of cluster **yields** from **FOPI** collaboration for $A \leq 4$

[R. Wang, Y.-G. Ma, L.-W. Chen, C. M. Ko, K.-J. Sun, & Z. Zhang, Phys. Rev. C 108, L031601 (2023)]

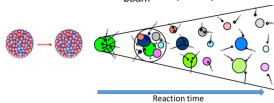
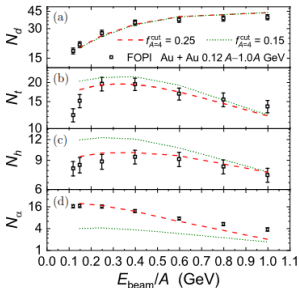


- Kinetic approach for HIC at intermediate energies
No α and ^3He & heavier fragments production
- Spinodal instability $\Rightarrow$ Mean-field (Vlasov) dynamics
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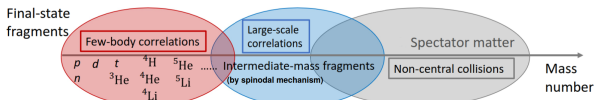
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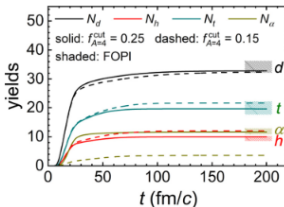
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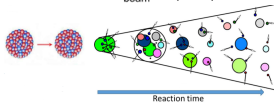
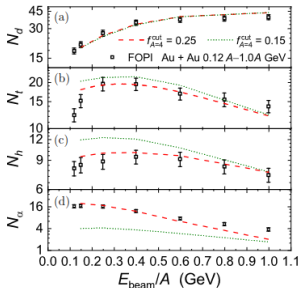
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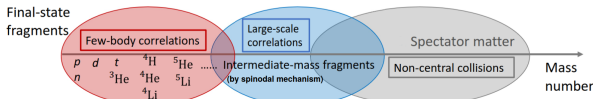
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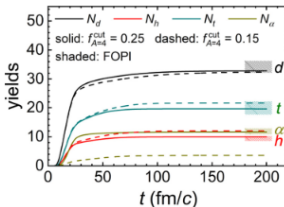
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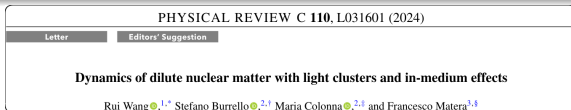
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Our goal

Assess if light **clusters**
(from **compression** phase)
affect **spinodal** instability
(**expansion** stage)

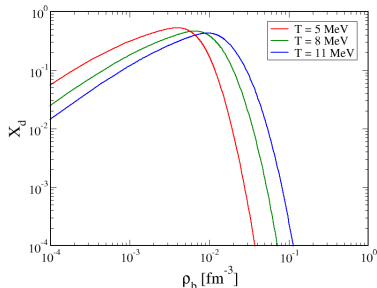
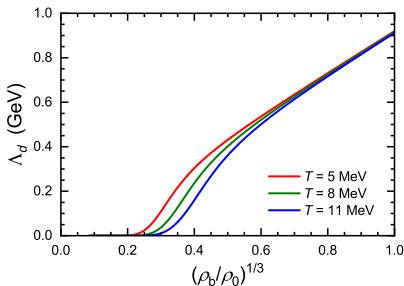
Density-dependent (Mott) momentum cut-off



- Pauli-blocking $\Rightarrow$ **Cut-off** (Mott) momentum $P_j^{\text{Mott}} \equiv \Lambda_j(\rho_b, T)$ parameterization

$$\rho_j = g_j \int_{|\mathbf{p}| > \Lambda_j} \frac{d\mathbf{p}}{(2\pi\hbar)^3} f_j \quad j = n, p, d \quad (\Lambda_q = 0, \text{ for } q = n, p)$$

- Chemical **equilibrium** $\Rightarrow X_d = \frac{A_d \rho_d}{\rho_0}$ **consistent** with microscopic calculations



Linearized Vlasov equations for NM+deuterons

- Linear response to **collision-less** Boltzmann $\Rightarrow$ linearized **Vlasov** equations for NMd

$$\partial_t (\delta f_j) + \nabla_{\mathbf{r}} (\delta f_j) \cdot \nabla_{\mathbf{p}} \varepsilon_j - \nabla_{\mathbf{p}} f_j \cdot \nabla_{\mathbf{r}} (\delta \varepsilon_j) = 0 \quad \Rightarrow \quad \delta \rho_j = -\chi_j \sum_l \left(F_0^{jl} + \tilde{F}_{\lambda}^{jl} \right) \delta \rho_l - \delta_{jd} \sum_l \Phi_{\lambda}^{dl} \delta \rho_l$$

- Single-particle energy $\varepsilon_j \equiv \frac{\delta \mathcal{E}}{\delta f_j(\mathbf{p})}$ (from **EDF** $\mathcal{E} = \mathcal{K} + \mathcal{U}$)

$$\varepsilon_j = \frac{p^2}{2m_j} + U_j + \tilde{\varepsilon}_j^{\lambda} \quad (\tilde{\varepsilon}_j^{\lambda} \propto \Phi_{\lambda}^{dj} \sim \frac{\partial \Lambda_d}{\partial \rho_j})$$

- Momentum-independent **Skyrme**-like interaction (= for bound and free nucleons)

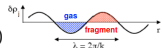
$$\mathcal{U} = \frac{A}{2} \frac{\rho_b^2}{\rho_0} + \frac{B}{\alpha + 2} \frac{\rho_b^{\alpha+2}}{\rho_0^{\alpha+1}} + \frac{C(\rho)}{2} \frac{\rho_3^2}{\rho_0} + \frac{D}{2} (\nabla_{\mathbf{r}} \rho_b)^2 - \frac{D_3}{2} (\nabla_{\mathbf{r}} \rho_3)^2$$

- Density-dependent** (Mott) momentum **cut-off** $\Rightarrow$ extra-terms in both $\delta \rho_j$ and ε_j

$$\rho_j = g_j \int_{|\mathbf{p}| > \Lambda_j} \frac{d\mathbf{p}}{(2\pi\hbar)^3} f_j \quad j = n, p, d \quad \rightarrow \quad \delta \rho_j(\mathbf{r}, t) = g_j \int_{|\mathbf{p}| > \Lambda_j} \frac{d\mathbf{p}}{(2\pi\hbar)^3} \delta f_j - \delta_{jd} \sum_{l=n,p,d} \Phi_{\lambda}^{dl} \delta \rho_l$$

- $\Phi_{\lambda}^{dl} \neq 0 \Rightarrow$ adding **in-medium** effects for cluster appearance/dissolution in **dynamics**

- Landau** procedure $\left(F_0^{jl} \sim \frac{\partial U_j}{\partial \rho_l}, \tilde{F}_{\lambda}^{jl} \sim \frac{\partial \tilde{\varepsilon}_j^{\lambda}}{\partial \rho_l} \right)$ for $\delta f_j \sim \sum_{\mathbf{k}} \delta f_j^{\mathbf{k}} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}$



Dispersion relation and spinodal instability region

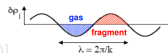
- Solving linearized Vlasov equations $\Rightarrow$ **dispersion relation** $\omega = \omega(k)$

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- $\omega = \text{Im}(\omega) \Leftrightarrow$ **unstable** mode (spinodal region)

[R. Wang, S. Burrello, M. Colonna, F. Matera, PRC 110, L031601 (2024)]

- $\omega = 0$ ($\chi_j = 1$) $\Rightarrow$ **border**
- $\text{Im}(\omega) \Rightarrow$ **growth rate**



Dispersion relation and spinodal instability region

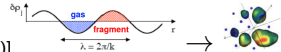
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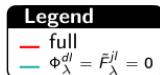
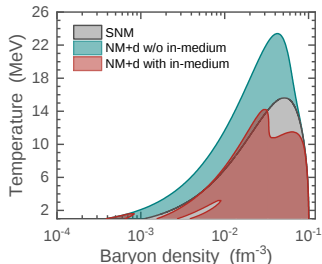
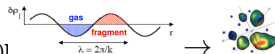
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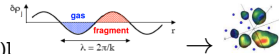
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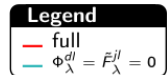
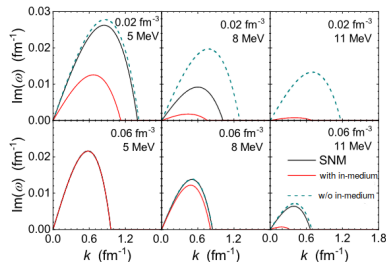
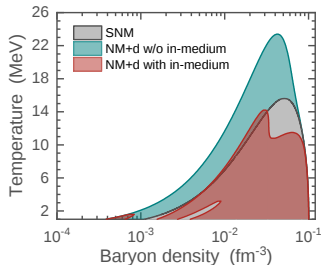
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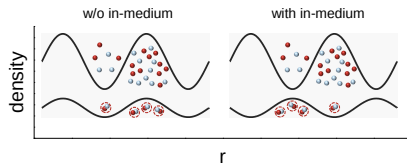
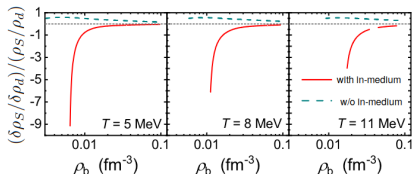


In-medium effects in dynamics

- **Slowdown** of instability rate & different **fragmentation** modes

Instability direction: “distillation” mechanism

- **Direction of instability** in space of density fluctuations: $\frac{\delta\rho_S}{\delta\rho_d} (\rho_S = \rho_n + \rho_p)$
- $\frac{\delta\rho_S}{\delta\rho_d} \geq 0 \Rightarrow$ **Nucleons** and **deuterons** fluctuations move in (out) of phase



[R. Wang, S. Burrello, M. Colonna, F. Matera, PRC 110, L031601 (2024)]

- **NMd with no in-medium effects:**
 - **Favored growth** of instabilities
 - **Cooperation** to form fragments
- **NMd with in-medium effects:**
 - Deuterons move to **low densities**
 - They might be **separately** emitted
 $\Rightarrow$ “**distillation**” mechanism

Outline of the presentation

① Many-body (MB) correlations and clustering phenomena in nuclear systems

- Understanding Equation of State (EOS) for nuclear matter (NM)
- Phenomenological models based on energy density functionals (EDF)

② Extended EDF-based models: recent developments and results

- Extended Skyrme and Gogny EDFs
- Cluster degrees of freedom
- Clusterization in heavy-ion collisions
- Clusterization in neutron stars

③ Further developments and outlooks

- Connection between hydrodynamical and linearized Vlasov approach
- Extensive numerical calculations of the dynamics with light clusters
- Consistent description of fragment formation mechanisms in heavy-ion collisions

④ Summary

Further developments and outlooks

● Hydrodynamics vs linearized Vlasov approach

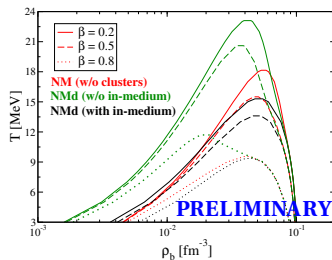
[S. Burrello et al., in preparation]

● Interplay ($d + \alpha$) & different cut-off

[Carmelo Piazza's Master's Thesis work]

● Microscopic description from in-medium SE

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Further developments and outlooks

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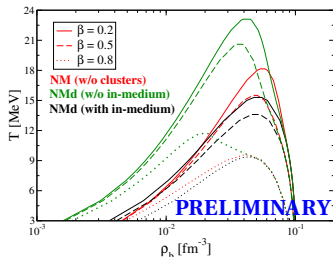
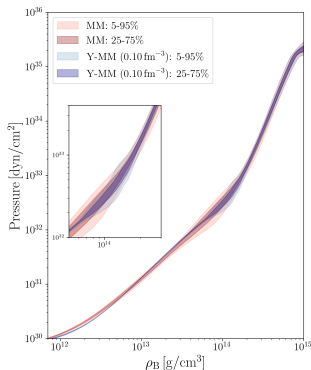
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Work in progress

- Implementation within transport simulations
- Connection with Bayesian methods

PHYSICAL REVIEW C **112**, 035802 (2025)

Bayesian inference of neutron star crust properties using an *ab-initio*–benchmarked metamodel

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(Received 6 June 2025; revised 23 July 2025; accepted 8 August 2025; published 5 September 2025)

- ## 4 Summary

Final remarks and conclusions

Main topic

- Description of **correlations** & **clustering** with phenomenological **EDF** models
- **Dynamics** of **dilute NM** with light **clusters** DOF and local **in-medium** effects

Main results

- Unified **mass-shift** parametrization for deuterons & **SRCs** and impact on **EOS**
- **Validation** of **phase-space excluded-volume** approach against **in-medium SE**
- Role of clusters on SNM **spinodal** instability and **fragmentation** dynamics

Further developments and outlooks

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- Extension to **ANM** with other light clusters and **cut-off** parameterizations
- **Numerical** calculations & **consistent** description of **HIC** fragment formation

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THANK YOU FOR YOUR ATTENTION!