ERC EXOTIC workshop - Frontiers in Nuclear Physics, November 21-23, 2023, Bonn

Ab initio study of nuclear clustering in hot dilute nuclear matter

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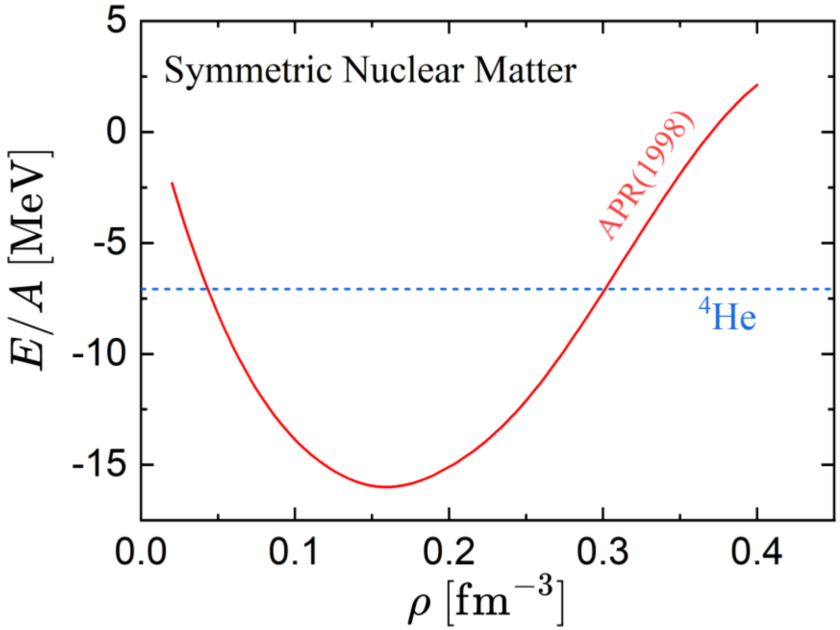
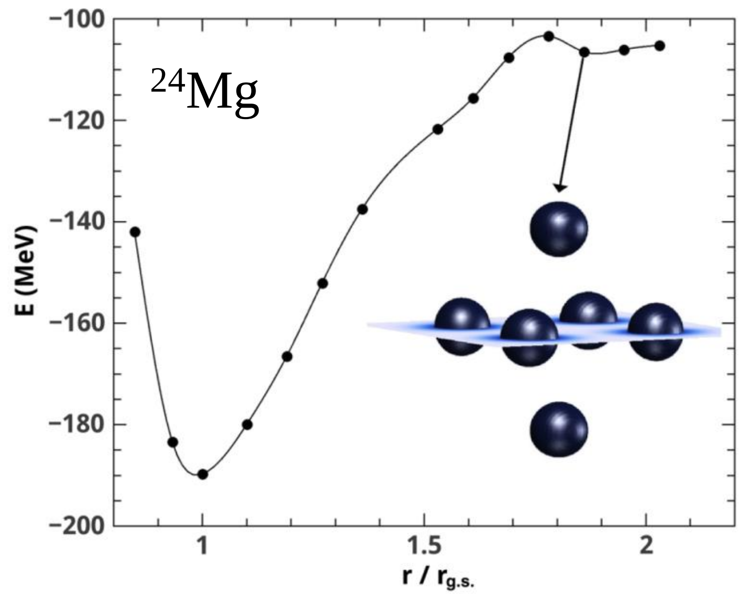
Nuclear clustering at subsaturation density

- Nuclear matter at subsaturation density can minimize its energy by forming clusters.



Akmal, Pandharipande, Ravenhall, PRC 58, 1804 (1998)



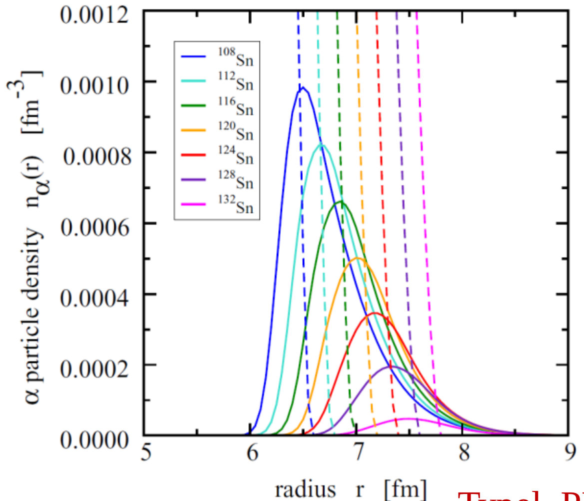
Girod, Schuck, PRL 111, 132503 (2013)

- Subsaturation density could be realized in many situations
  - Astrophysical object, like neutron star and core-collapse supernova
    Janka, Langanke, Marek, Martínez-Pinedo, Müller, Phys. Rep. 442, 38 (2007)
  - Heavy-ion collisions Qin et al., PRL 108, 172701 (2012); Pais *et al.*, PRL 125, 012701 (2020)

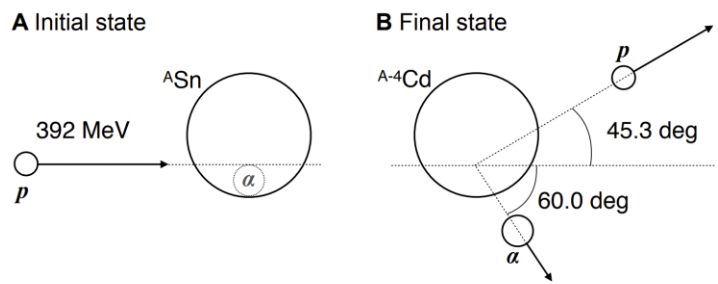
- Recent works indicate it also relates to the alpha formation in heavy nuclei.

Alpha formation in heavy nuclei

- Alpha formation in the surface of heavy nuclei

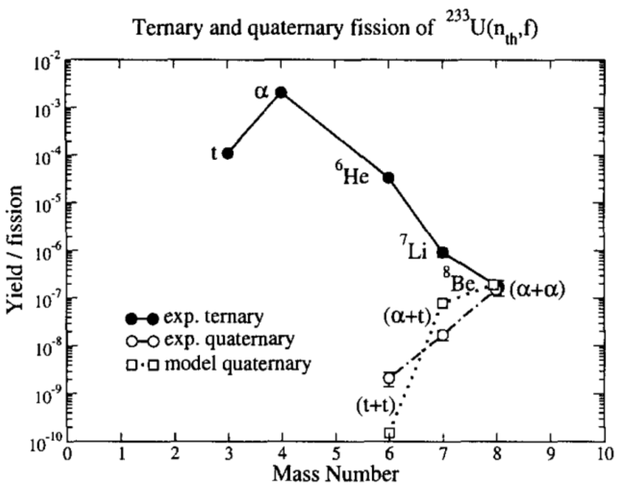


Typel, PRC 89, 064321 (2014)

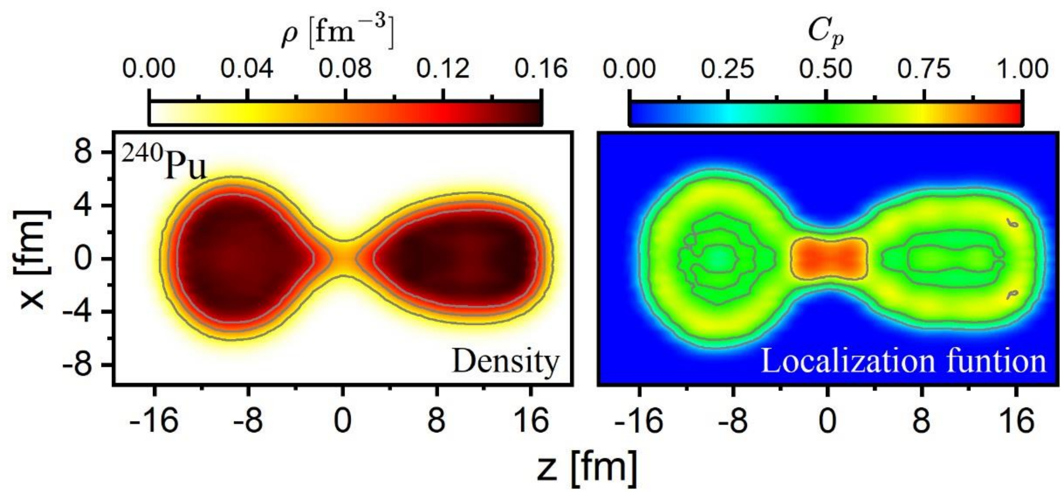


Tanaka *et al.*, Science 371, 260 (2021)

- Alpha formation in ternary and quaternary fission



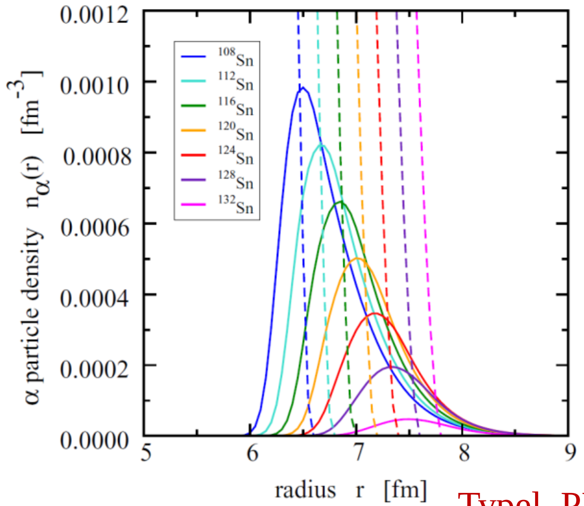
F. Gönnenwein, Nucl. Phys. A 734, 213 (2004)



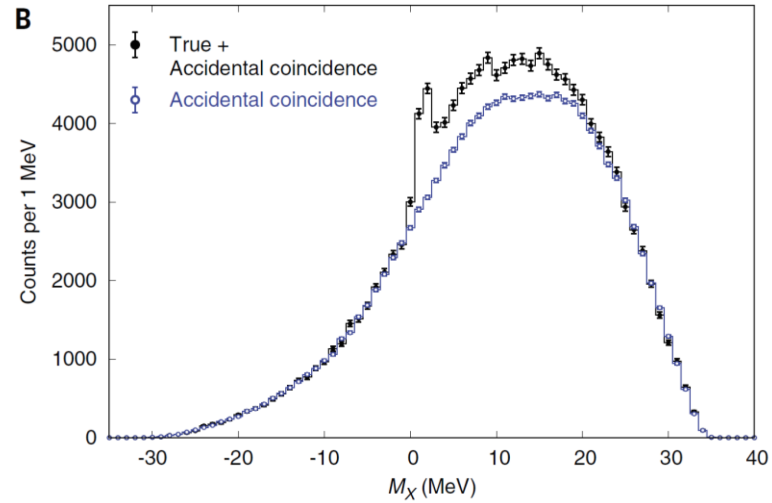
ZXR, Vretenar, Nikšić, Zhao, Zhao, Meng, PRL 128, 172501 (2022)

Alpha formation in heavy nuclei

- Alpha formation in the surface of heavy nuclei

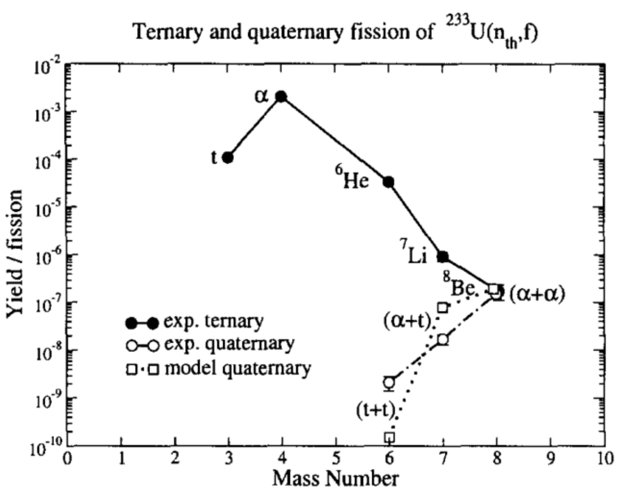


Typel, PRC 89, 064321 (2014)

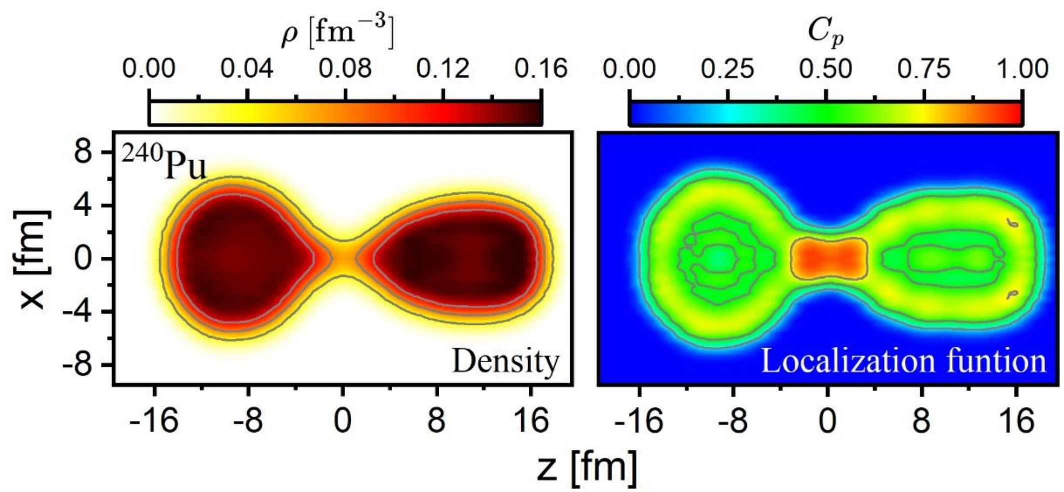


Tanaka *et al.*, Science 371, 260 (2021)

- Alpha formation in ternary and quaternary fissions



F. Gönnenwein, Nucl. Phys. A 734, 213 (2004)



ZXR, Vretenar, Nikšić, Zhao, Zhao, Meng, PRL 128, 172501 (2022)

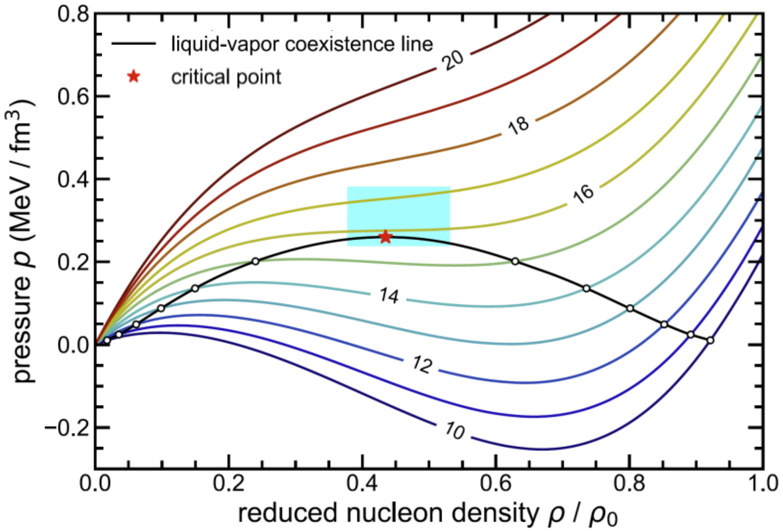
Theoretical description for hot dilute nuclear matter

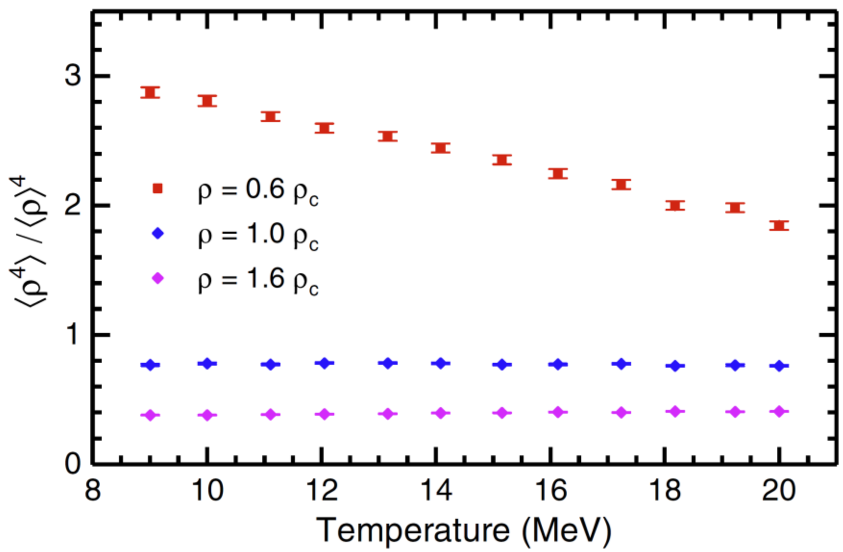
- A valid treatment of the **nuclear clustering in low density matter** is important to understand the property of dilute nuclear matter.
- Various methods on the nuclear clustering of hot dilute nuclear matter
  - Virial expansions Horowitz, Schwenk, NPA 776, 55 (2006)
  - Mean-field theory combined other method, e.g., Thomas-Fermi approximation Shen, Toki, Oyamatsu, Sumiyoshi, NPA 637, 435 (1998)
  - Quantum statistical approach Röpke, Schulz, Münchow, NPA 379, 536 (1982)
  - Generalized relativistic mean-field model Typel, Röpke, Klähn, Blaschke, Wolter, PRC 81, 015803 (2010)
  - Transport models A. Ono, PPNP 105, 139 (2019)
  - …
- However, there have been no **ab initio calculations** to address this subject.
- Challenges on ab initio calculations
  - Method designed for thermodynamic calculations
  - Inclusion of the nuclear clustering involving strong many-body correlations

NLEFT for nuclear thermodynamics

- Nuclear lattice effective field theory (NLEFT) could include nonperturbative effects such as nuclear clustering.
- Recently, it was extended to calculations of the thermodynamics of nuclear systems using the pinhole trace algorithm.

Lu, Li, Elhatisari, Lee, Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)





In this work, the species and abundances of nuclear clusters in hot dilute nuclear matter will be investigated based on NLEFT.

Partition function in lattice space

- For a system with nucleon number A and temperature $T(=1/\beta)$, the expectation of an observable could be expressed via partition function $Z(\beta)$,

$$\langle \mathcal{O} \rangle_\beta = \frac{Z_{\mathcal{O}}(\beta)}{Z(\beta)} = \frac{\mathrm{Tr}_A(e^{-\beta H}\mathcal{O})}{\mathrm{Tr}_A(e^{-\beta H})}$$

with $\mathrm{Tr}_A(\cdots)$ the trace over the A-nucleon states $\{|\phi_k\rangle\}$,

$$\mathrm{Tr}_A(\cdots) = \sum_k \langle \phi_k | \cdots | \phi_k \rangle$$

- In lattice space, a natural choice for $|\phi_k\rangle$ is the Slater determinants composed of point particles,

$$|\phi_k\rangle = |c_1, c_2, \cdots, c_A\rangle$$

where $c_i = (\boldsymbol{n}_i, \sigma_i, \tau_i)$ are the quantum numbers for i-th particle.

- Partition function $Z(\beta)$ could be expressed as,

$$Z(\beta) = \sum_{c_1,\cdots,c_2} \langle c_1, \cdots, c_A | e^{-\beta H} | c_1, \cdots, c_A \rangle \equiv \sum_{\vec{c}} \langle \vec{c} | e^{-\beta H} | \vec{c} \rangle$$

Transfer matrix with auxiliary field

- Set $\beta = L_t a_t$: split β into L_t slices with temporal spacing a_t

$$e^{-\beta H} = (: e^{-a_t H} :)^{L_t} \equiv M^{L_t}$$

- Lattice Hamiltonian with SU4 symmetric interaction:

$$H = K + \frac{C_2}{2} \sum_{\boldsymbol{n}} : \tilde{\rho}^2(\boldsymbol{n}) : + \frac{C_3}{6} \sum_{\boldsymbol{n}} : \tilde{\rho}^3(\boldsymbol{n}) :$$

with smeared density operator,

$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^{+}(\boldsymbol{n}) \tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^{+}(\boldsymbol{n}') \tilde{a}_i(\boldsymbol{n}'),$$

$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}')$$

- Expansion with auxiliary field Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, PLB 797, 134863 (2019)

$$: \exp\left(-\frac{a_t C_2}{2} \tilde{\rho}^2 - \frac{a_t C_3}{6} \tilde{\rho}^3\right) : = \sum_{k=1}^{3} \omega_k : \exp\left[\sqrt{-a_t C_2}\, s_k \tilde{\rho}\right] :$$

- Transfer matrix with auxiliary field

$$M(s) = \int \mathcal{D}s : \exp\left[-a_t K + \sqrt{-a_t C_2} \sum_{\boldsymbol{n}} s(\boldsymbol{n}) \tilde{\rho}(\boldsymbol{n})\right] :$$

Pinhole trace algorithm

- The partition function with auxiliary field

$$Z_{\mathcal{O}}(\beta) = \sum_{\vec{c}} \int \mathcal{D}s_1 \cdots \mathcal{D}s_{L_t} \langle \vec{c}| \, M(s_{L_t}) \cdots M(s_{L_t/2+1}) \, \mathcal{O} \, M(s_{L_t/2}) \cdots M(s_1) |\vec{c}\rangle$$

$$Z(\beta) = \sum_{\vec{c}} \int \mathcal{D}s_1 \cdots \mathcal{D}s_{L_t} \langle \vec{c}| \, M(s_{L_t}) \cdots M(s_{L_t/2+1}) M(s_{L_t/2}) \cdots M(s_1) |\vec{c}\rangle$$

- In pinhole trace algorithm, $Z(\beta)$ and $Z_{\mathcal{O}}(\beta)$ are evaluated using importance sampling. The ensemble Ω of $\{\vec{s}, \vec{c}\}$ is generated according to probability distribution,

$$P(\vec{s}, \vec{c}) = |\langle \vec{c}| M(s_{L_t}) \cdots M(s_1) |\vec{c}\rangle|$$

- The expectation of an observable could be written as,

$$\langle \mathcal{O} \rangle = Z_{\mathcal{O}}(\beta)/Z(\beta) = \langle \mathcal{M}_{\mathcal{O}}(\vec{s}, \vec{c}) \rangle_{\Omega} / \langle \mathcal{M}_1(\vec{s}, \vec{c}) \rangle_{\Omega}$$

where

$$\mathcal{M}_{\mathcal{O}}(\vec{s}, \vec{c}) = \langle \vec{c}| M(s_{L_t}) \cdots M(s_{L_t/2+1}) \, \hat{O} \, M(s_{L_t/2}) \cdots M(s_1) |\vec{c}\rangle / P(\vec{s}, \vec{c})$$

- To generate the ensemble Ω, $\vec{s}$ and $\vec{c}$ are updated alternately.

Lu, Li, Elhatisari, Lee, Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)

Correlation functions for nuclear clustering

- The clustering in nuclear matter can be regarded as a spatial localization of nucleons.
- Correlation functions to measure nucleon localization:

$$G_{11}(n) = L^3 \sum_{\{\sigma_i \tau_i\}} : \rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(\boldsymbol{n}) :$$

$$G_{21}(n) = L^3 \sum_{\{\sigma_i \tau_i\}} : \rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(0)\rho_{\sigma_3\tau_3}(\boldsymbol{n}) :$$

$$G_{31}(n) = L^3 \sum_{\{\sigma_i \tau_i\}} : \rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(0)\rho_{\sigma_3\tau_3}(0)\rho_{\sigma_4\tau_4}(\boldsymbol{n}) :$$

$$G_{22}(n) = L^3 \sum_{\{\sigma_i \tau_i\}} : \rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(0)\rho_{\sigma_3\tau_3}(\boldsymbol{n})\rho_{\sigma_4\tau_4}(\boldsymbol{n}) :$$

where $\sum_{\{\sigma_i \tau_i\}}$ denotes summation over all spin-isospin indices without a repetition,

$$\sum_{\{\sigma_i \tau_i\}} \equiv \sum_{\sigma_1\tau_1} \sum_{\sigma_2\tau_2} \cdots \prod_{i<j} (1 - \delta_{\sigma_i\tau_i,\sigma_j\tau_j})$$

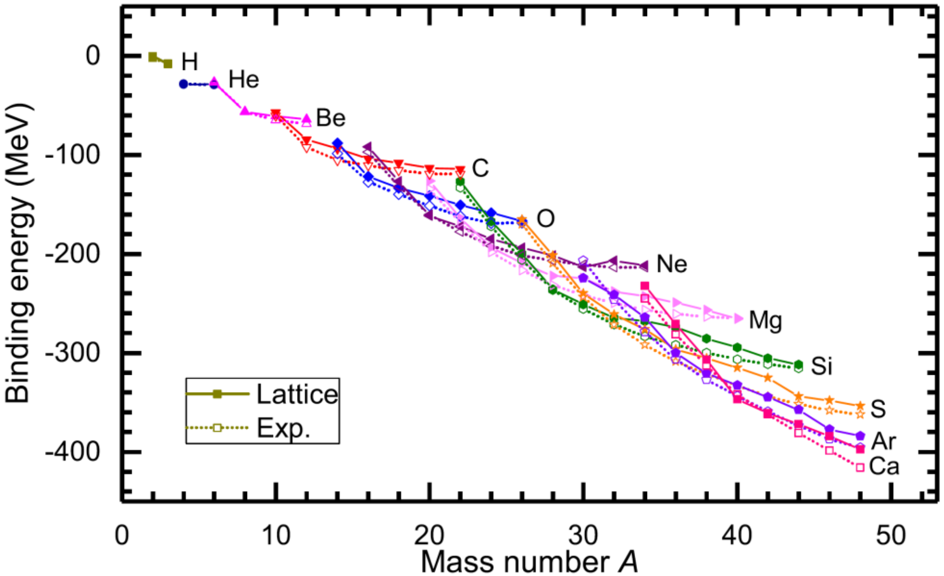
In the case of $G_{11}(n)$, it reads

$$\sum_{\{\sigma_i \tau_i\}} \equiv \sum_{\sigma_1\tau_1} \sum_{\sigma_2\tau_2} (1 - \delta_{\sigma_1\tau_1,\sigma_2\tau_2})$$

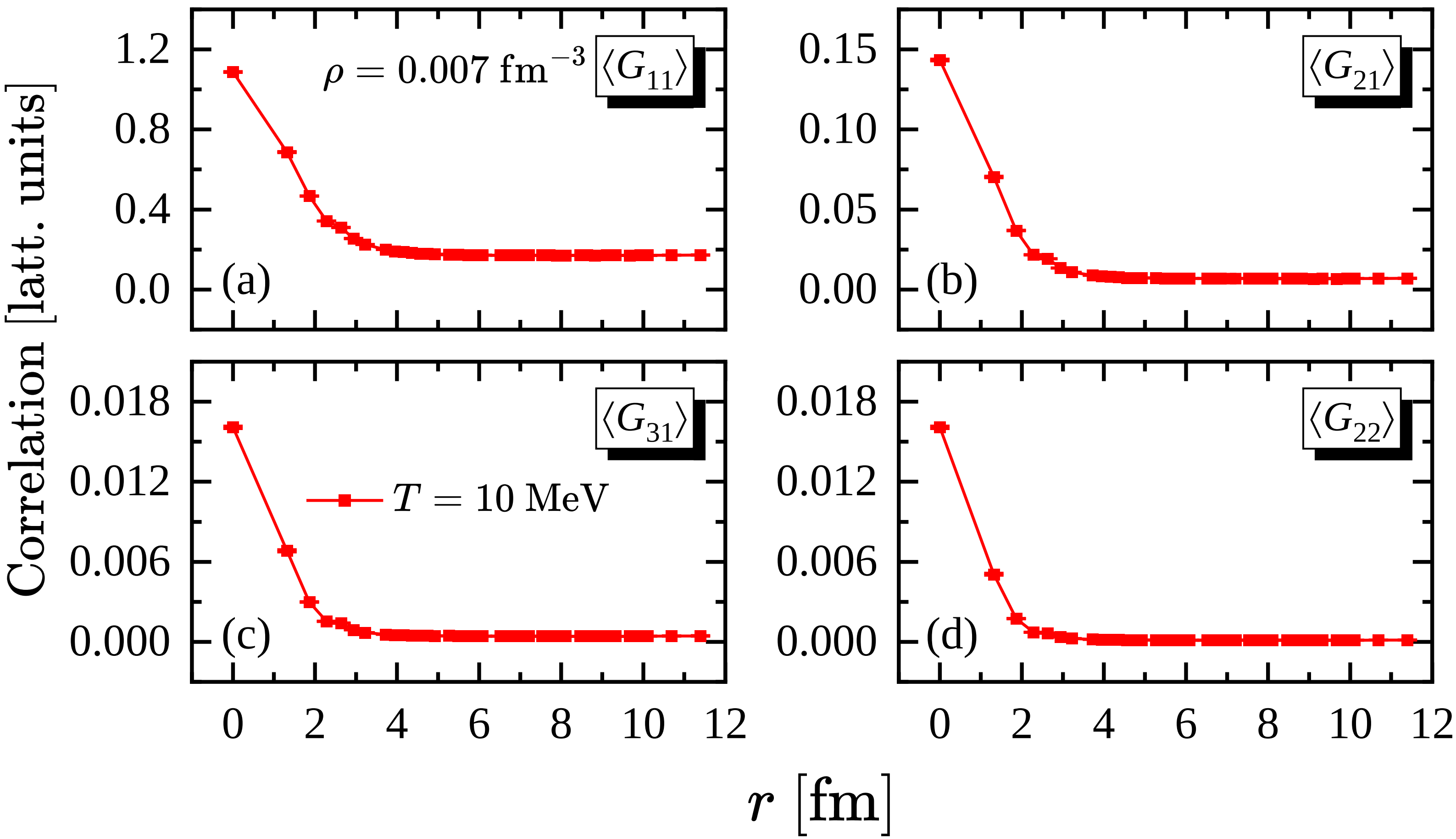
ZXR, Elhatisari, Lähde, Lee, Meißner, arXiv:2305.15037

Numerical details

- **Spatial lattice spacing:** $a = 1.32$ fm
- **Temporal lattice spacing:** $a_t = 1/2000\ \mathrm{MeV}^{-1}$
- **Box size:** $L = 10$ (if not specified)
- **Boundary condition:** twisted boundary conditions
- **Low energy constants:** Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, PLB 797, 134863 (2019)
  - $C_2 = -3.41 \times 10^{-7}\ \mathrm{MeV}^{-2}$, $C_3 = -1.4 \times 10^{-14}\ \mathrm{MeV}^{-5}$
  - $s_L = 0.5$, $s_{NL} = 0.061$



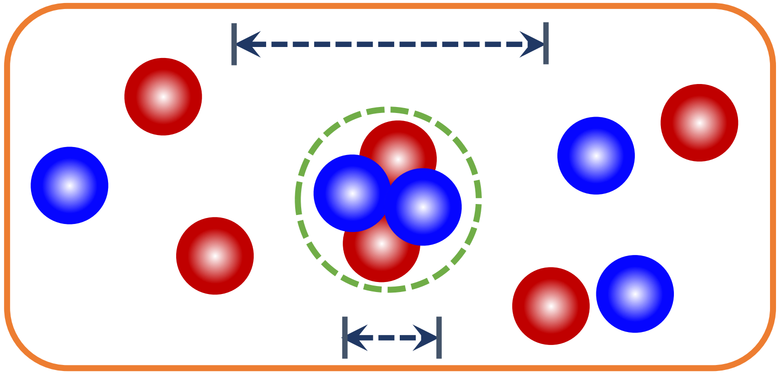
$G_{ij}(n)$ with ρ = 0.007 fm^{-3} and T = 10 MeV



ZXR, Elhatisari, Lähde, Lee, Meißner, arXiv:2305.15037

- **Short range:** strong peak ⇒ Evidence of nuclear clustering
- **Long range:** flat curve with nonzero value ⇒ System is a gas of nucleons and clusters

Light-cluster distillation



- *A single cluster* contributes predominantly to short-range correlations.
- *Two nucleons or clusters* contribute to both long-range and long-range correlations.

- **Light-cluster distillation**
  - Assume that the clusters are dominated by light clusters such as dimers (^{2}H, *nn*, *pp*), trimers (^{3}He,^{3}H), and tetramers (^{4}He).
  - The correlation functions are expanded by individual light clusters,

$$\langle G_{11}(n)\rangle \approx \langle G_{11}^{l}\rangle + w_4\langle G_{11}(n)\rangle_4 + w_3\langle G_{11}(n)\rangle_3 + w_2\langle G_{11}(n)\rangle_2$$

$$\langle G_{21}(n)\rangle \approx \langle G_{21}^{l}\rangle + w_4\langle G_{21}(n)\rangle_4 + w_3\langle G_{21}(n)\rangle_3$$

$$\langle G_{31}(n)\rangle \approx \langle G_{31}^{l}\rangle + w_4\langle G_{31}(n)\rangle_4$$

$$\langle G_{22}(n)\rangle \approx \langle G_{22}^{l}\rangle + w_4\langle G_{22}(n)\rangle_4$$

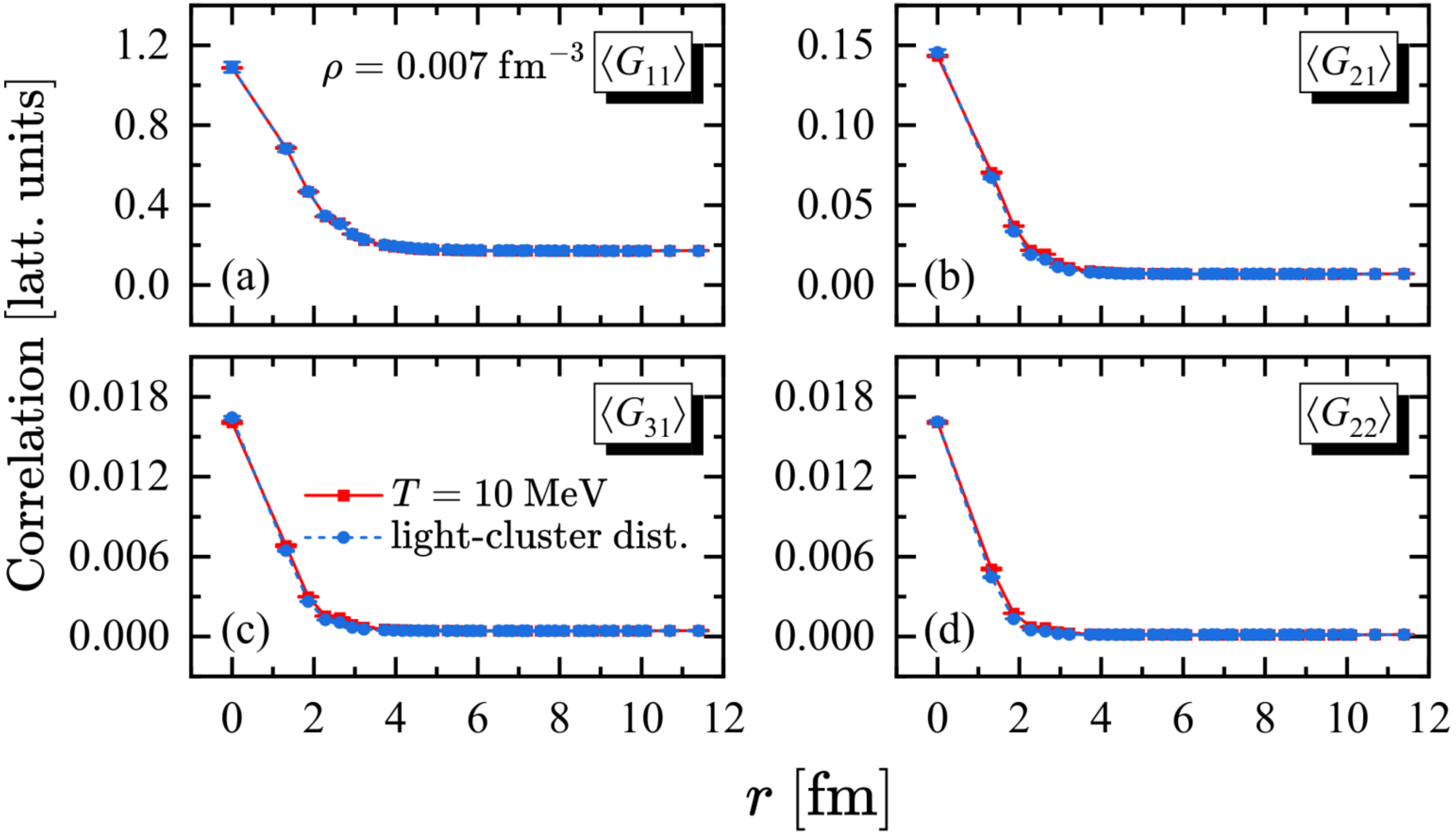
where G_{ij}^{l} denotes the long-range parts of the correlation functions.

  - Physical interpretation of w_2, w_3, w_4: the average numbers of light clusters.

ZXR, Elhatisari, Lähde, Lee, Meißner, arXiv:2305.15037

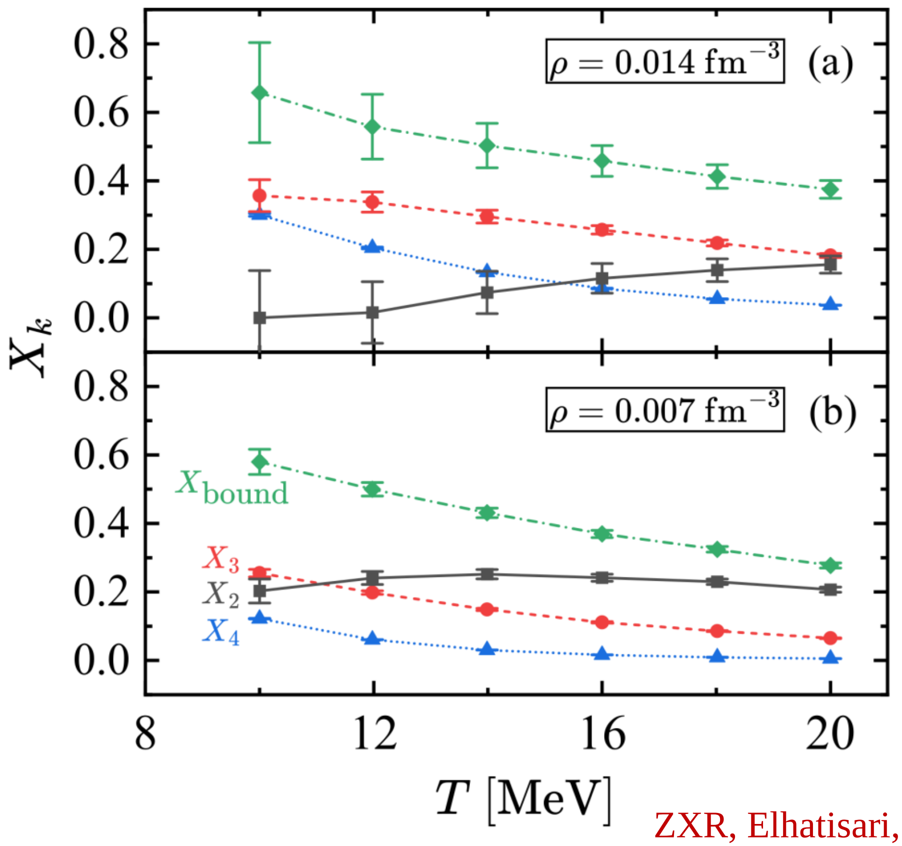
Light-cluster distillation

- Four correlations are well reproduced with only three parameters.



- Cluster numbers: $w_2 = 1.62 \pm 0.28$, $w_3 = 1.36 \pm 0.06$, $w_4 = 0.49 \pm 0.01$
- Mass fractions: $X_k = kw_k/A$, $X_{\mathrm{bound}} = X_2 + X_3 + X_4$

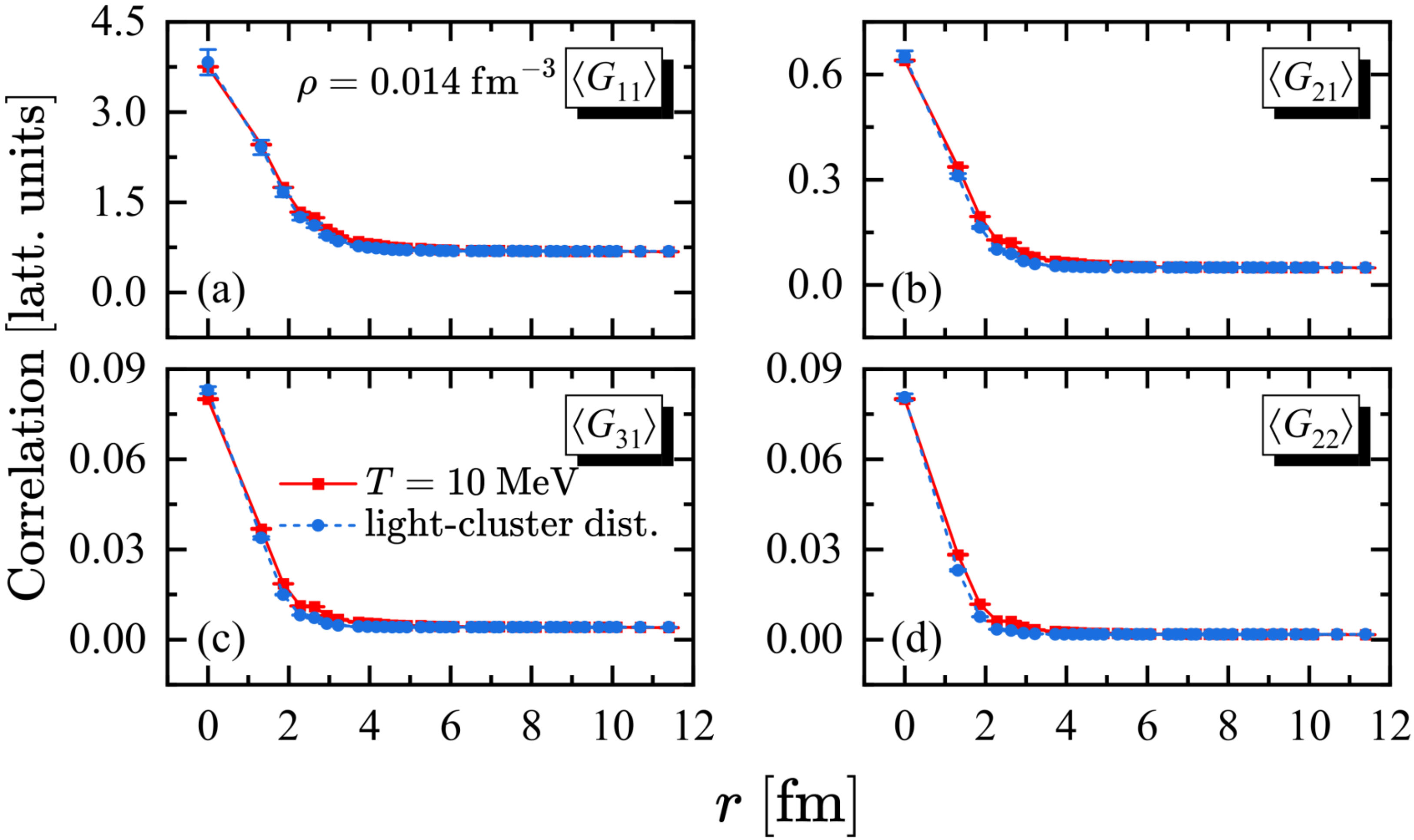
Mass fractions $X_k(\rho, T)$



ZXR, Elhatisari, Lähde, Lee, Meißner, arXiv:2305.15037

- The decreases of X_{bound} with T: thermal evaporation of nucleons from the clusters.
- **Fixed $\boldsymbol{\rho}$:** X_3 and X_4 decrease with T, while X_2 is slightly increasing or relatively flat.
- **Fixed $\boldsymbol{T}$:** X_3 and X_4 increase with ρ, while X_2 is decreasing.
- Why are the fitting uncertainties at $\rho = 0.014\ \mathrm{fm}^{-3}$ and $T = 10$ MeV so large?

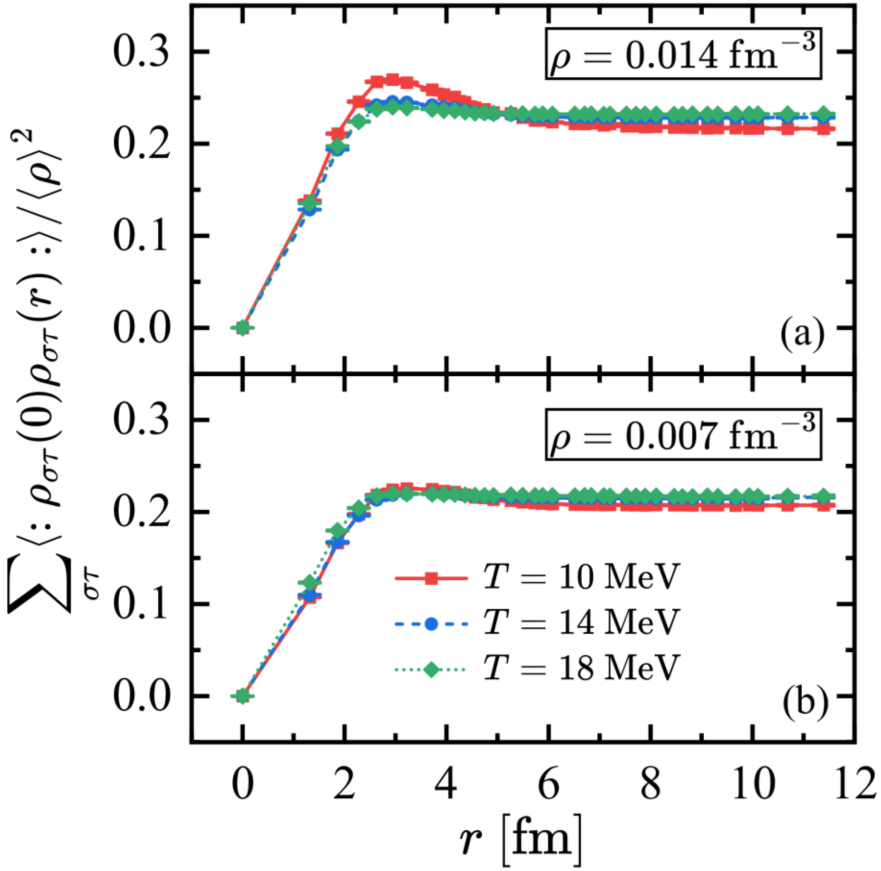
$G_{ij}(n)$ with ρ = 0.014 fm^{-3} and T = 10 MeV



- The deviation of light-cluster distillation from $T = 10$ MeV become a little larger.
- *Is this caused by heavier clusters with A>4?*

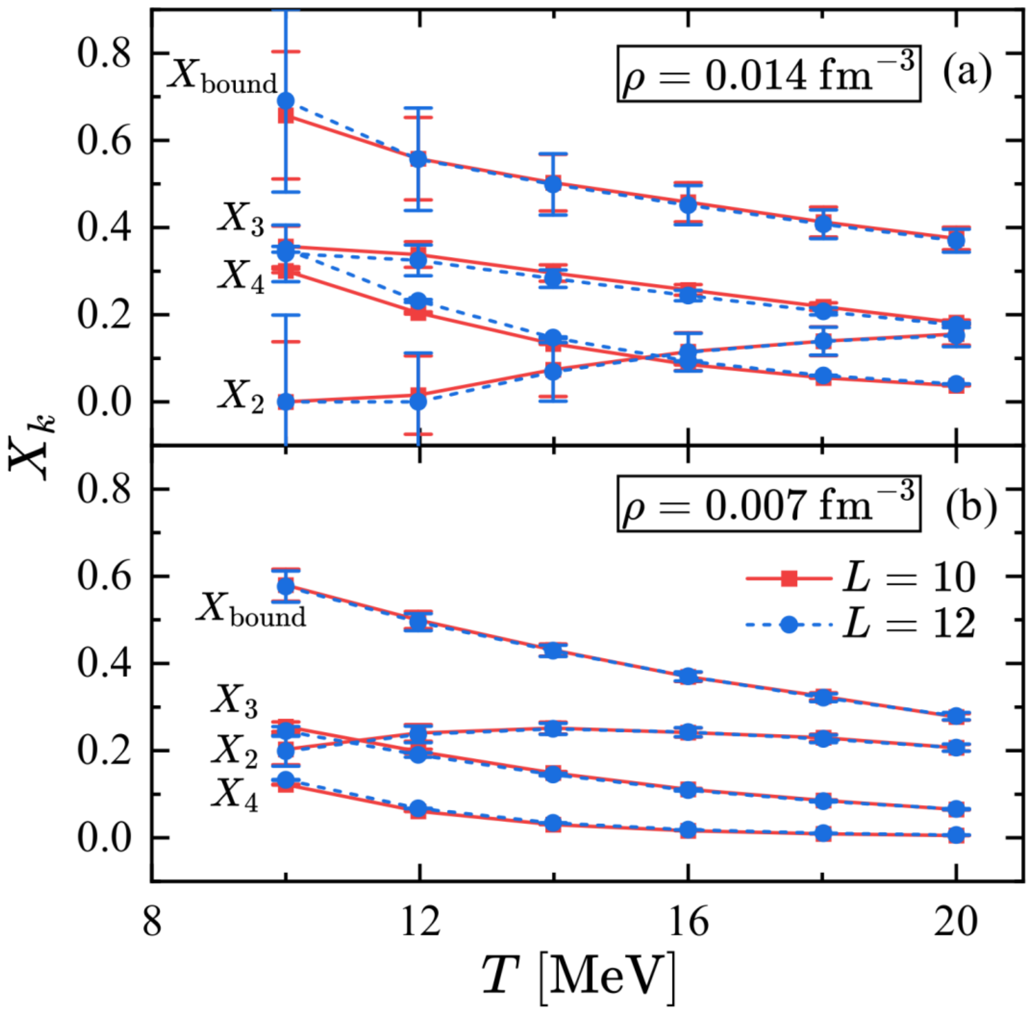
Correlation function with same spin and isospin

- Heavier cluster with $A > 4$ would induce spatial localizations of two nucleons with the same spin and isospin.



- The peak at $\rho = 0.014\ \mathrm{fm}^{-3}$ and $T = 10$ MeV provides a direct evidence for the emergence of heavier clusters.

Finite volume effects



Total particle number

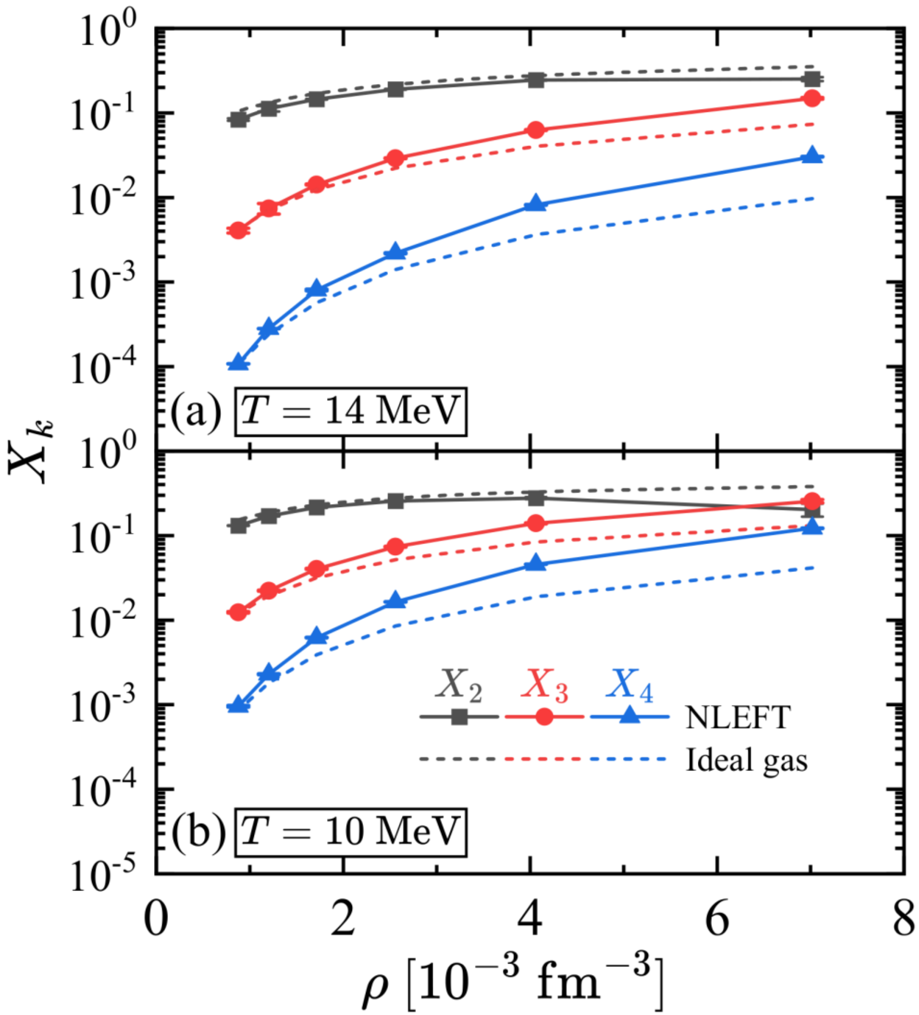
ρ [fm^{-3}]	$L = 10$ (13.2 fm)	$L = 12$ (15.8 fm)
0.007	16	28
0.014	32	56

The results with $L = 10$ and 12 are nearly the same.

- Thermal wavelength $\lambda = \sqrt{2\pi/(mT)} = 3\sim5$ fm is much smaller than box size 13.2 fm.
- Twisted boundary conditions accelerate the convergence to the thermodynamic limit

Comparison with ideal gas model

- **Ideal gas model:** grand canonical ensemble



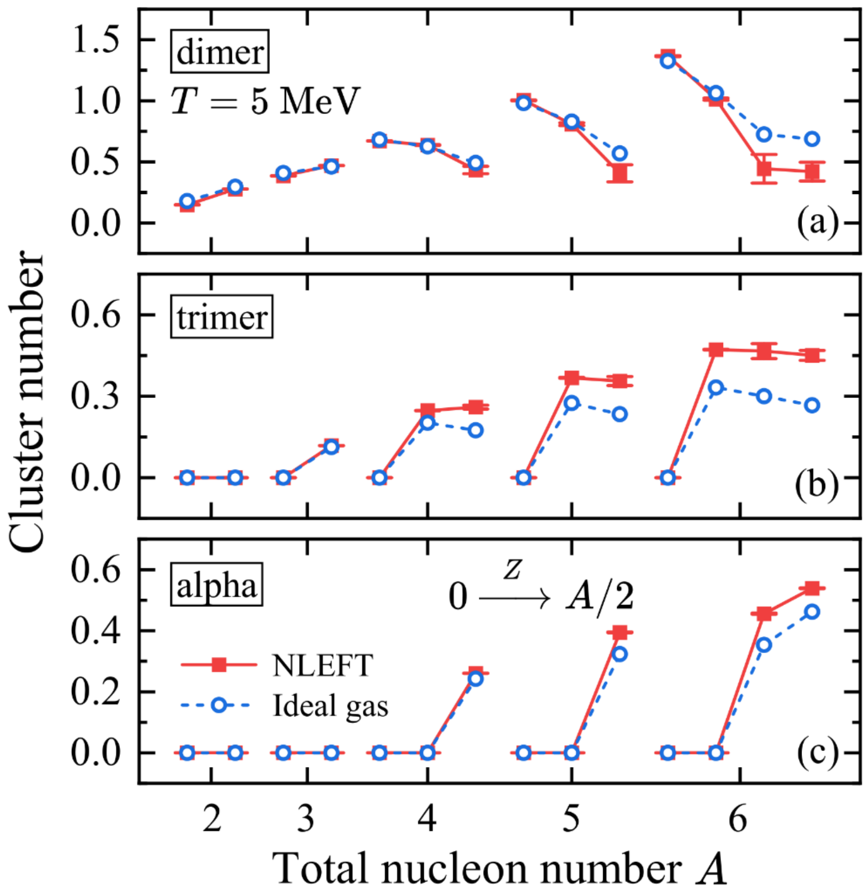
- From left to right, particle number $A = 16$ with $L = 20, 18, \ldots, 10$.
- Heavier clusters are negligible.

✓ At low density around $\rho \approx 0.001\ \mathrm{fm}^{-3}$, the agreement is excellent for all clusters.

✓ Notable deviations appear with approaching $\rho \approx 0.007\ \mathrm{fm}^{-3}$.

Comparison with ideal gas model

- **Ideal gas model:** canonical ensemble



Dimer:

- No significant deviation with $Z \leq 1$; n-n, n-p, n-np, n-nn, nn-nn, nn-np interactions have no significant impact on dimer abundance.
- Notable deviations with $Z \geq 2$; nn-pp or np-np interactions reduce the dimer abundance.

Trimer and tetramer (alpha):

✓ Noticeable differences first appear at $A = 4, Z = 2$ (trimer) and $A = 5, Z = 2$ (tetramer).

✓ Nucleon-trimer (nucleon-tetramer) interaction enhances trimer (tetramer) abundance.

Summary and Perspectives

☐ Summary

- Nuclear clustering in hot dilute nuclear matter are investigated based on NLEFT simulations.
- A theoretical framework *light-cluster distillation* is introduced to determine the species and abundances of light nuclear clusters.
- NLEFT results show an excellent agreement with ideal gas predictions at low densities around $\rho \simeq 0.001\ \mathrm{fm}^{-3}$. At higher densities, deviations from ideal gas abundances become larger due to cluster-nucleon and cluster-cluster interactions.

☐ Perspectives

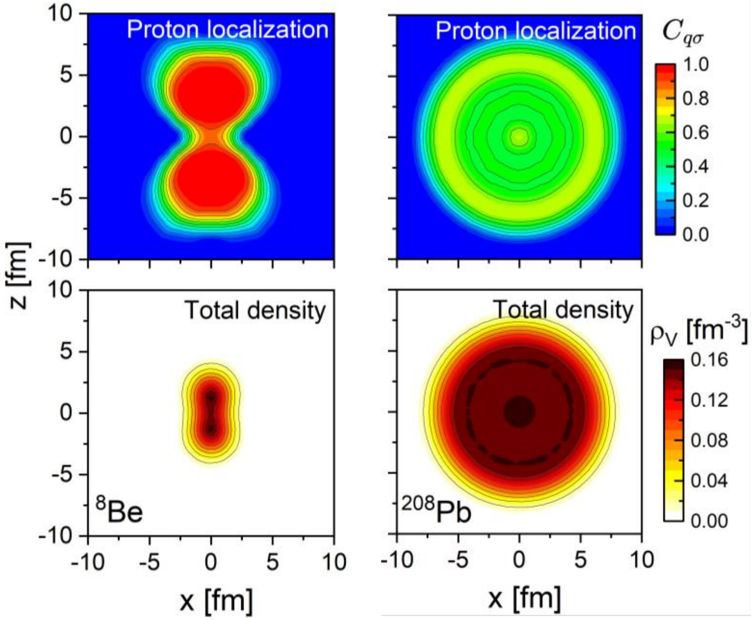
- Simulations with high-fidelity chiral interactions at N3LO. (in progress)
- Asymmetric nuclear with the comparison to experimental data.
- Go beyond light-cluster distillation to include heavier clusters.

THANK YOU!

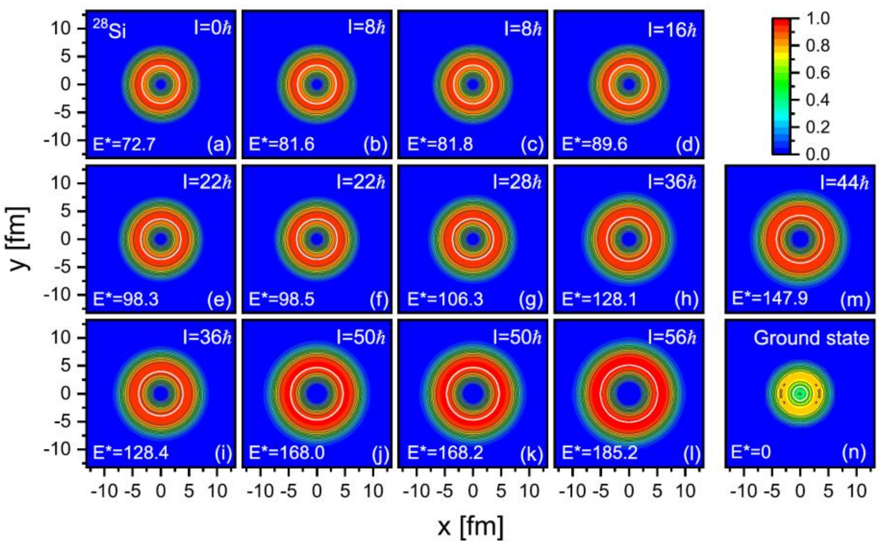
Nucleon localization function

- **Nucleon localization function** $C_{q\sigma}(\boldsymbol{r})$: Describe the likelihood two nucleon with same spin and isospin within a short distance
  - ✓ α cluster: $C_{q\sigma}(\boldsymbol{r}) \sim 1$, like ^{8}Be.
  - ✓ No localization: $C_{q\sigma}(\boldsymbol{r}) \sim 1/2$, like ^{208}Pb.

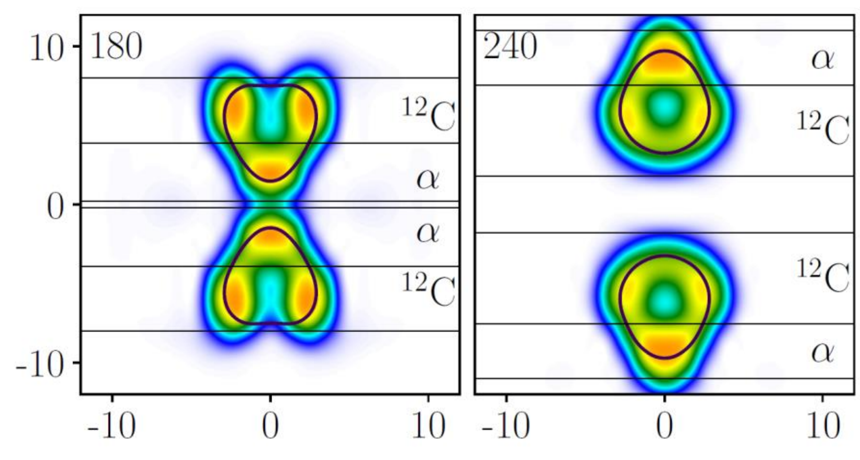
Reinhard, Maruhn, Umar, Oberacker, PRC 83, 034312 (2011)



- **Application in the nuclear cluster structure**



ZXR, Zhao, Zhang, Meng, NPA 996, 121696 (2020)



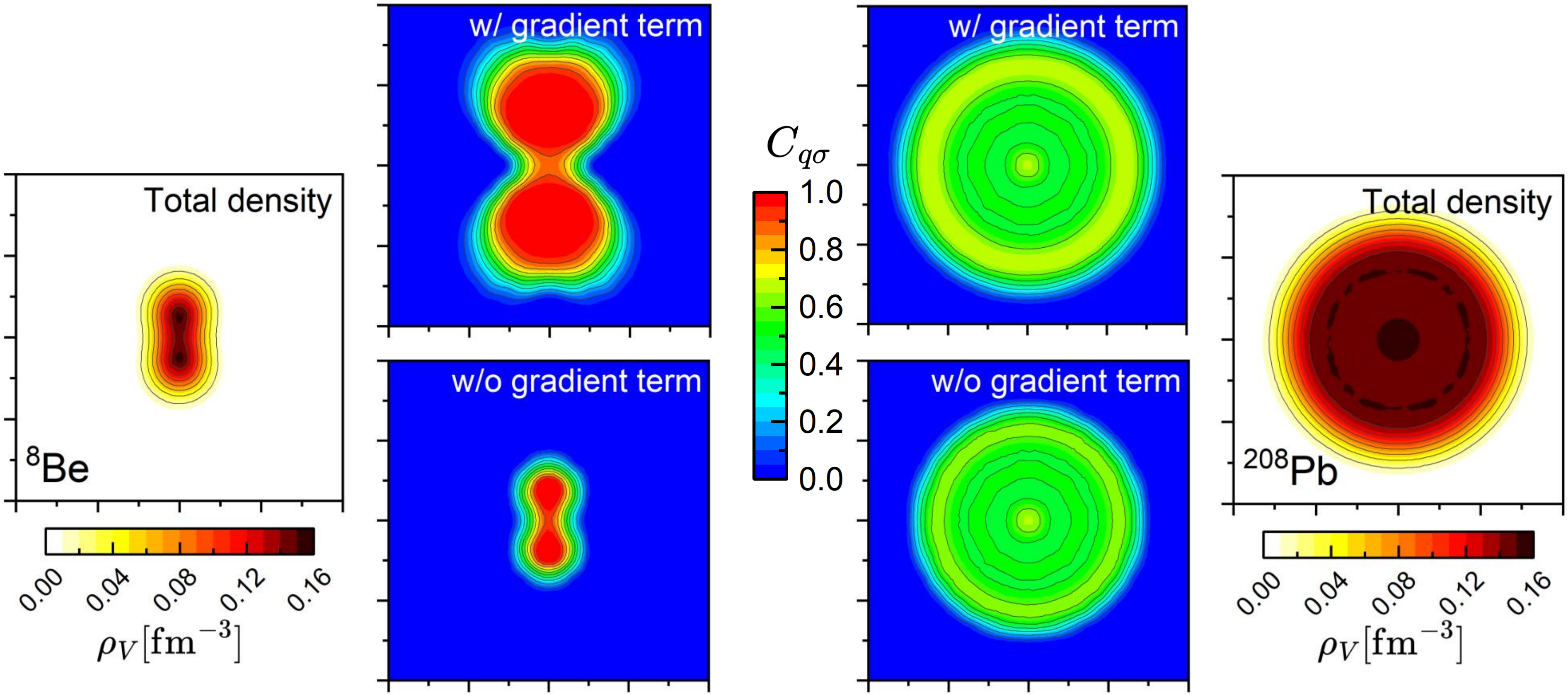
Schuetrumpf, Nazarewicz, PRC 96, 064608 (2017)

Impact of gradient term in nucleon localization function

Nucleon localization function: $C_{q\sigma}(\boldsymbol{r}) = \left\{1 + \left[D_{q\sigma}(\boldsymbol{r}) / \tau_{q\sigma}^{\mathrm{TF}}(\boldsymbol{r})\right]^2\right\}^{-1}$

$$D_{q\sigma}(\boldsymbol{r}) = \tau_{q\sigma}(\boldsymbol{r}) - \boxed{\frac{1}{4}\frac{|\boldsymbol{\nabla}\rho_{q\sigma}(\boldsymbol{r})|^2}{\rho_{q\sigma}(\boldsymbol{r})} - \frac{|\boldsymbol{j}_{q\sigma}(\boldsymbol{r})|^2}{\rho_{q\sigma}(\boldsymbol{r})}}$$

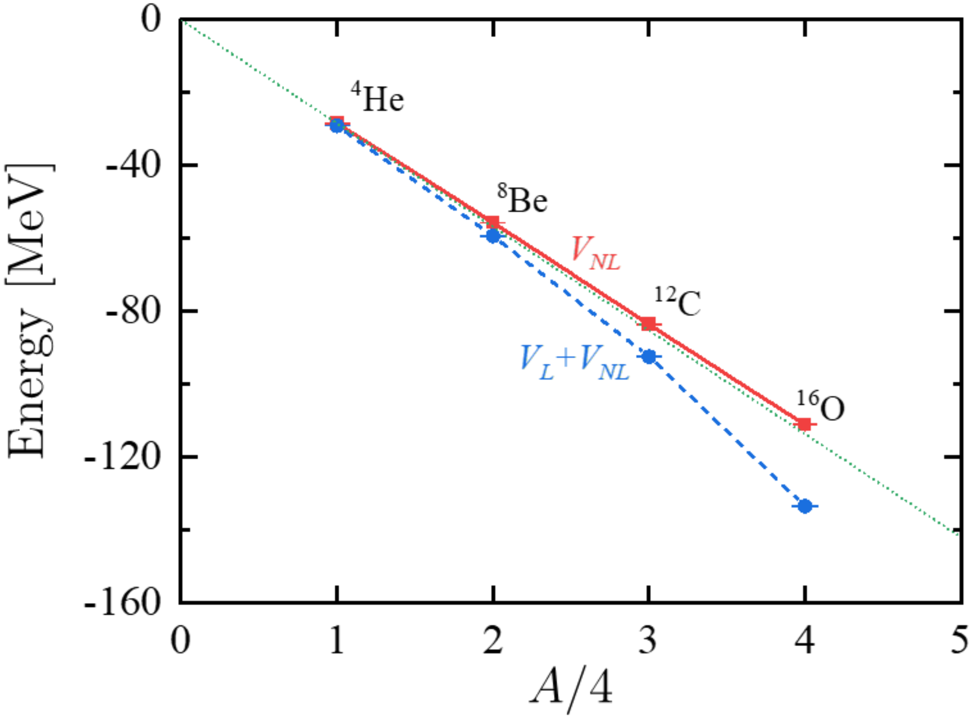
Neglected in Bulgac, Phys. Rev. C 108, L051303 (2023)



Pure nonlocal interaction

➢ **Low energy constants of pure nonlocal (NL) interaction:**

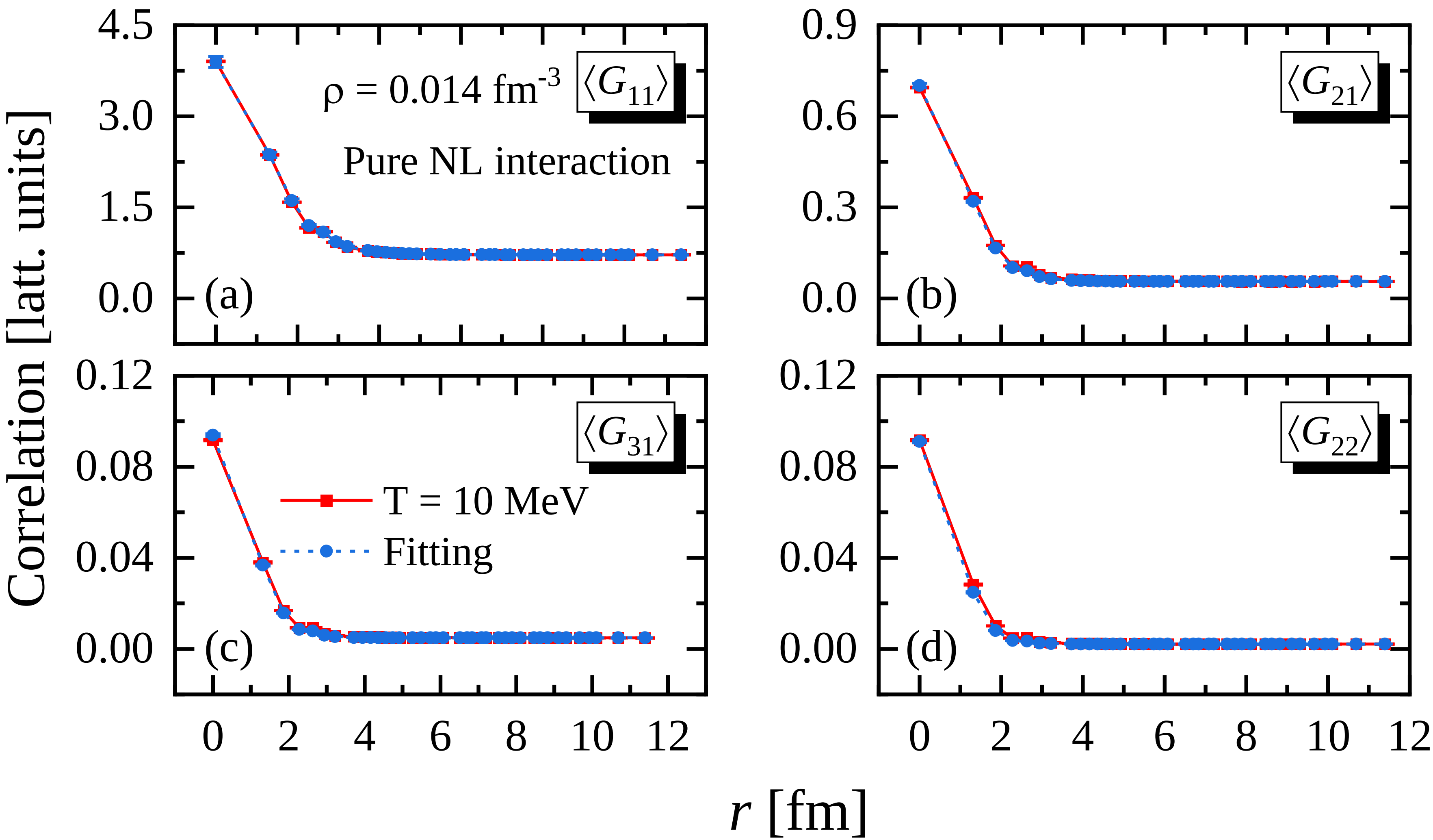
- $C_2 = -5.5 \times 10^{-7}\ \mathrm{MeV}^{-2}$, $C_3 = -1.4 \times 10^{-14}\ \mathrm{MeV}^{-5}$
- $s_L = 0.5$, $\boldsymbol{s_{NL} = 0}$



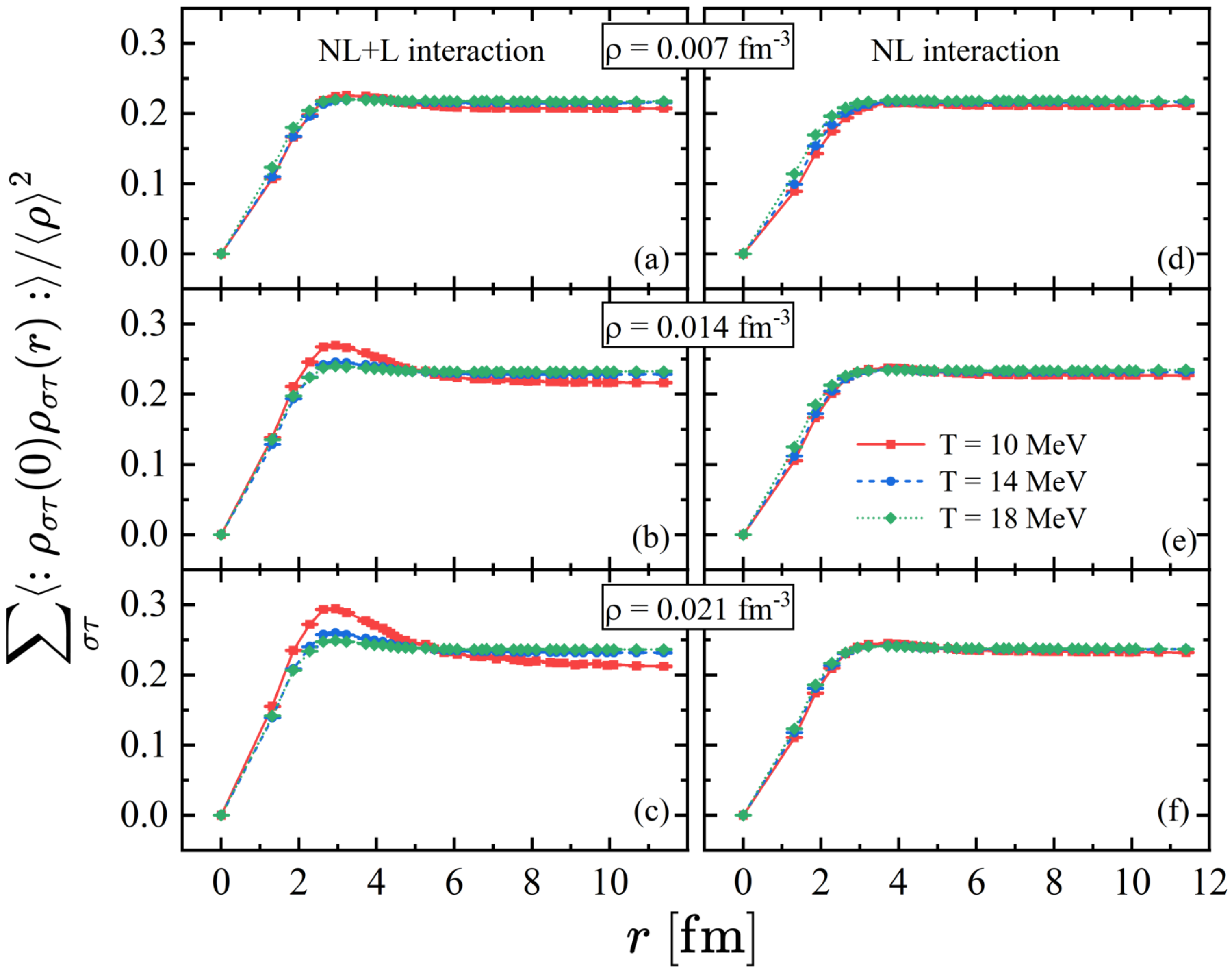
➢ These nuclei are systems of Bose-condensed gas of alpha particles.

Elhatisari et al. PRL 117, 132501 (2016)

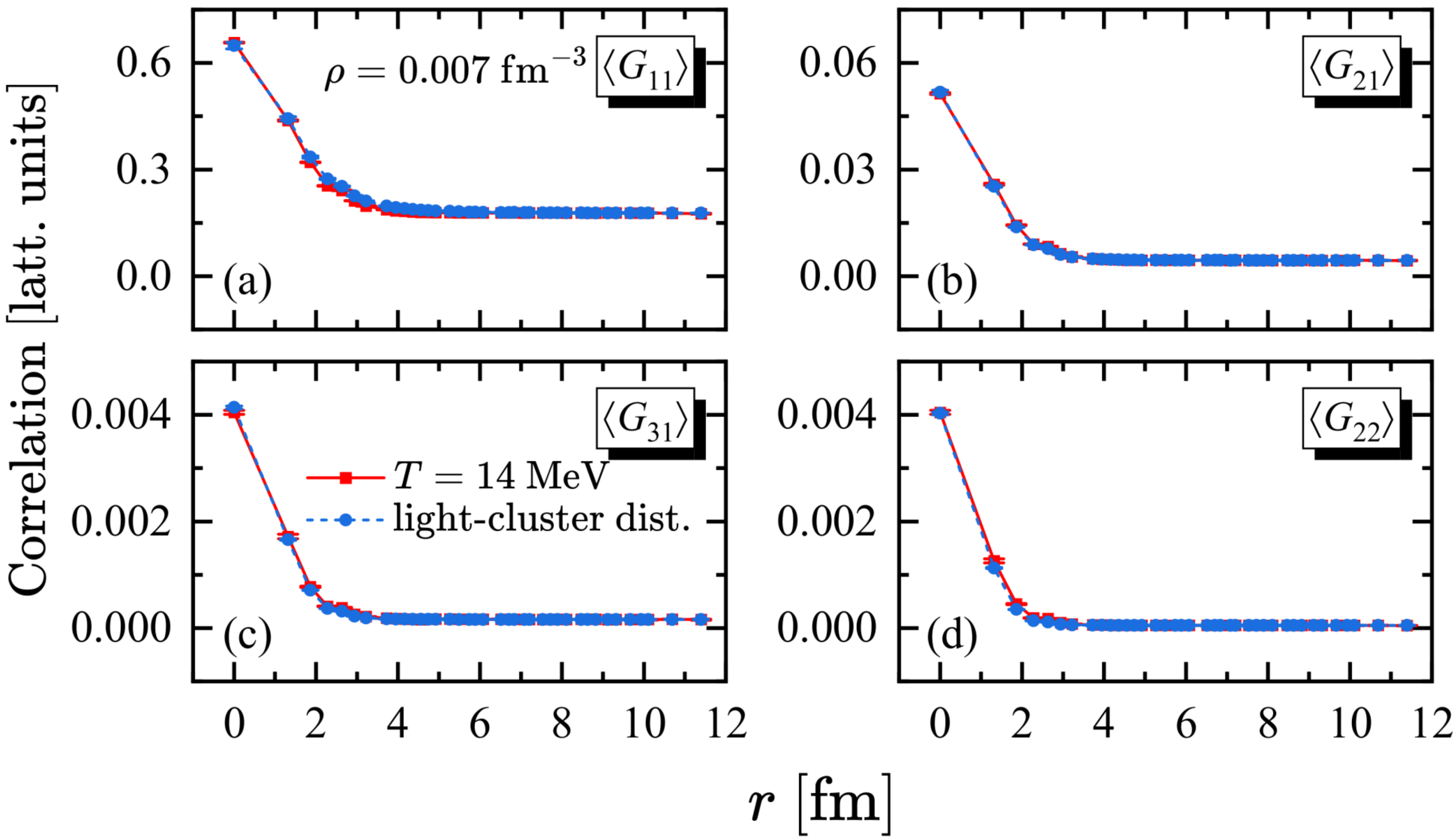
Pure nonlocal interaction



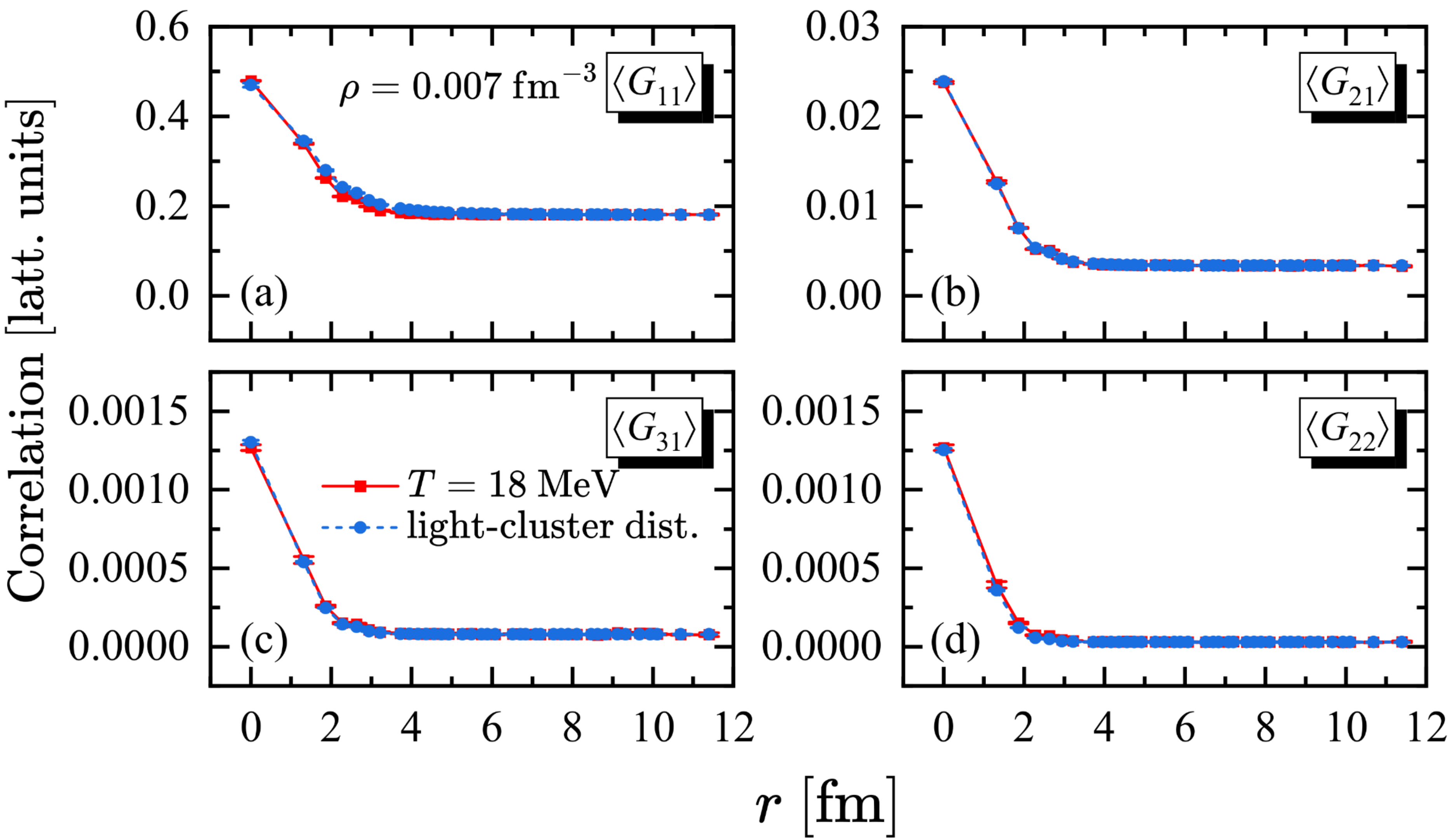
Correlation function with same spin and isospin



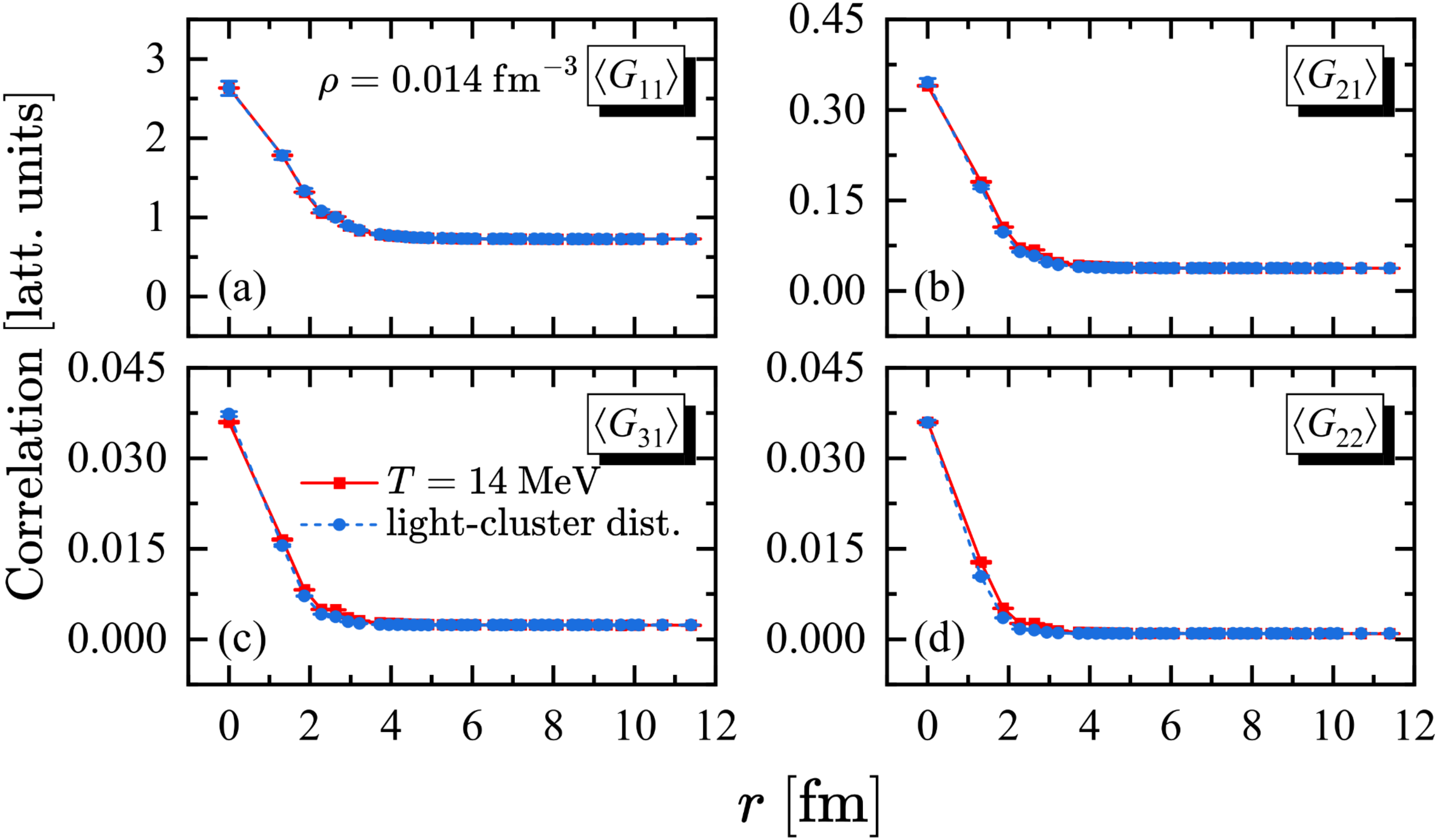
$G_{ij}(n)$ with ρ = 0.007 fm^{-3} and T = 14 MeV



$G_{ij}(n)$ with ρ = 0.007 fm^{-3} and T = 18 MeV



$G_{ij}(n)$ with ρ = 0.014 fm^{-3} and T = 14 MeV



$G_{ij}(n)$ with ρ = 0.014 fm^{-3} and T = 18 MeV