Nuclear Entanglement Entropy in terms of Short Range Correlations

2022 SRC Collaboration Meeting

August 4

Ehoud Pazy

Outline

<u>Brief Introduction:</u>

- What is entanglement entropy?
  - Area law
- Orbital Entanglement
- What has already been calculated for nuclear structure?
  - Neutron-Proton Entanglement entropy
  - ^{4}He and ^{6}He
- The General Contact Formalism (GCF) in a nutshell.

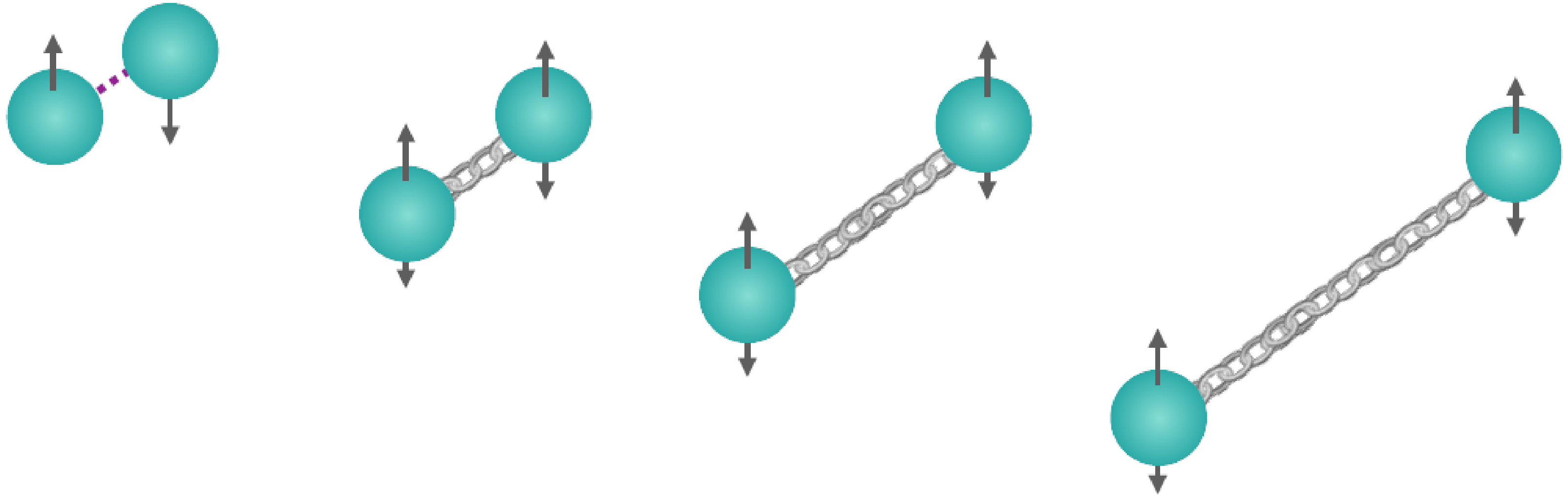
Outline

Calculating Entanglement Entropy for SRC:

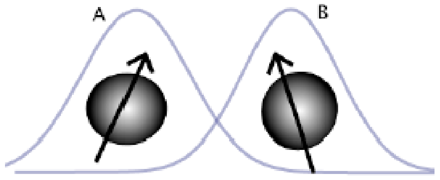
- Calculating the entanglement entropy of a single SRC pair.
- Summing up the Entanglement Entropy of SRC pairs.
- Comparing results with the ^{4}He calculations.
- Entropy from the single particle occupation.
- The Fermi Gas part.

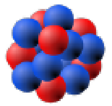
Entanglement

Entanglement describes the non-local, purely quantum correlations of a system



Entanglement at short distance, when particles have overlapping wave functions:



ex: nucleons in the nucleus 

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Entanglement Entropy

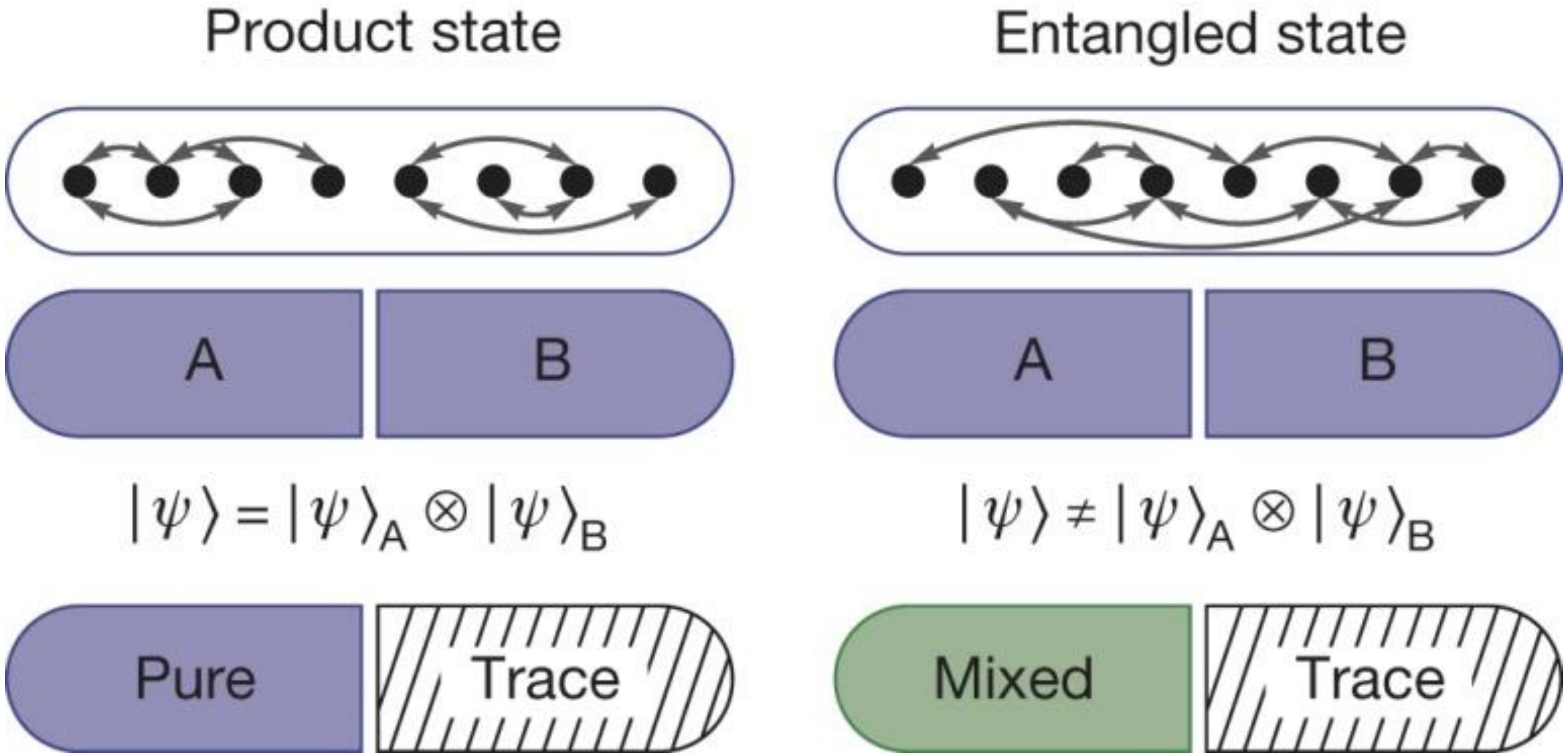
Is not a thermal entropy that originates
from a lack of knowledge about the microstate of the system.

Results from tracing out part of the system
This entropy arises because of the quantum correlations-Entanglement

Even at zero temperature we will encounter a non-zero entropy!

.

Entanglement Entropy:
Product verses Entangled



S=0

S>0

R Islam *et al.* *Nature* **528,** 78 (2015)

Definition of Entanglement Entropy

Divide a given quantum system into two parts A and B.
Then the total Hilbert space becomes factorized

$$H_{tot} = H_A \otimes H_B$$

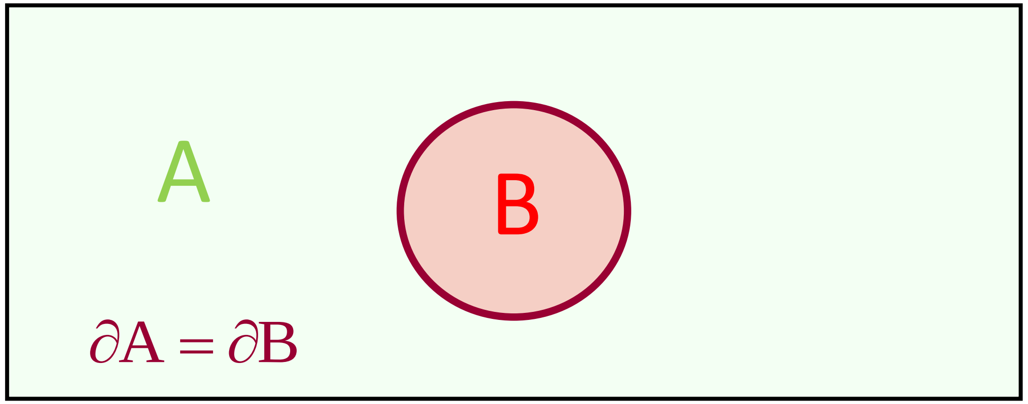
We define the reduced density matrix ρ_A for A by

$$\rho_A = \mathrm{Tr}_B \rho_{tot}$$

Tracing over the Hilbert space of B .
Now the entanglement entropy S_A is defined by the von Neumann entropy

$$S_A = -\mathrm{Tr}_A \, \rho_A \log \rho_A$$

Entangled Entropy Area Law



Expect that the entropy of a distinguished region B, be extensive
Such a behavior is referred to as a volume scaling and is observed for thermal states.

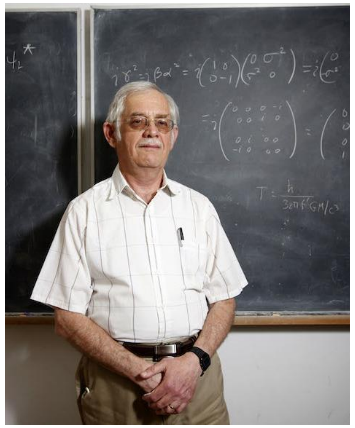
One typically finds an area law, or an area law with a small (often logarithmic) correction:
The scaling of the entropy of a region is merely linear in the boundary area of the region.

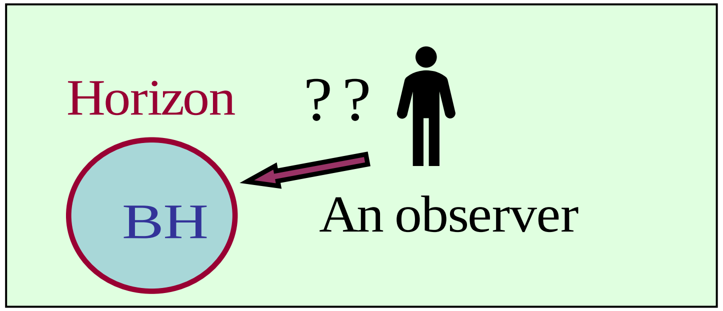
The Holographic Principle and Black Hole Entropy

The Bekenstein-Hawking entropy of a black hole which is proportional to its boundary surface.

The holographic principle—the conjecture that the information contained in a volume of space can be represented by a theory which lives in the boundary of that region—could be related to the area law behavior of the entanglement entropy in microscopic theories

An analogy with Black hole entropy





The boundary region $\partial A \sim$ the event horizon

Why is Entanglement Entropy Important?

Knowledge:

What role do genuine quantum correlations entanglement play in quantum many-body systems?

- It gives a measure of the correlations in the system. Specifically it is very useful to measure how entangled ground states are. An important measure is the entanglement entropy.
- Search for new order parameters

Applications:

- Quantum information and quantum computing.

Why is Entanglement Entropy Important?

Nuclear physics:

Is there a simple picture in which we can understand nuclear properties?

Is there an efficient scheme in which to model nuclear structure for applications?

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$\left|01101000...\right\rangle \left|10010100...\right\rangle$$

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Can we truncate for just a few components?

Computational Impossibility

Contributed talk FM 8 : Johnson

SAN DIEGO STATE UNIVERSITY

Despite advances, it is easy to get to model spaces beyond our reach:

shells between 50 and 82 ($0g_{7/2}$ 2s1d $0h_{11/2}$)

^{128}Te: dim 13 million (laptop)

^{127}I: dim 1.3 billion (small supercomputer)

^{128}Xe: dim 9.3 billion (supercomputer)

^{129}Cs: dim 50 billion (haven't tried!)

Computationally Important

$$|\Psi\rangle = \sum_{i_p,j_p} \Psi_{i_p,j_n} |i_p\rangle |j_n\rangle \longrightarrow |\Psi\rangle = \sum_{a,b} \tilde{\Psi}_{ab} |\pi_a\rangle |\nu_b\rangle$$

Initial Basis
Where the uncoupled basis states are Slater determinants

$$|\pi_a\rangle = \sum_{i_p} U^{\pi}_{ai_p} |i_p\rangle$$

Pure proton base

Goal $$|\Psi\rangle = \sum_{a,b=1}^{N} \tilde{\Psi}_{ab} |\pi_a\rangle |\nu_b\rangle, \quad N << \min(d_p, d_n)$$

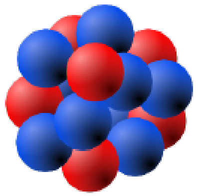
$$|\Psi\rangle = \sum_{\alpha} c_\alpha |\Phi_\alpha\rangle \qquad 1 = \sum_{\alpha} |c_\alpha|^2$$

d_p and d_n are the number of proton and neutron basis

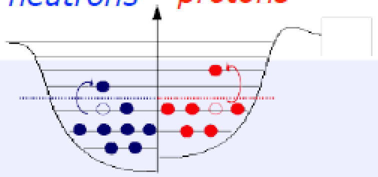
The weights tell us how much we can truncate.

Master Thesis, Oliver Gorton , 2018

Entanglement in the Nucleus



= Z protons + N neutrons



$$|\Psi\rangle = \sum_{\pi\nu} C_{\pi\nu} |\phi_\pi\rangle \otimes |\phi_\nu\rangle$$

$$= \sum_{n_{\pi_1} n_{\pi_2} \dots n_{\nu_1} n_{\nu_2} \dots} C_{n_{\pi_1} n_{\pi_2} \dots n_{\nu_1} n_{\nu_2} \dots} |n_{\pi_1} n_{\pi_2} \dots n_{\nu_1} n_{\nu_2} \dots\rangle$$

occupation numbers $n_i = 0 \text{ or } 1$

$$n_{\pi_1} + n_{\pi_2} \dots + n_{\nu_1} + n_{\nu_2} \dots = Z + N$$

Several types of entanglement are present in the nucleus:

✳ Entanglement between proton and neutron subsystems (distinguishable)

see e.g.: Papenbrock & Dean PRC 67, 051303(R) (2003), in the framework of DMRG;
Gorton & Johnson (Gorton Master thesis 2018), in the traditional Shell Model

✳ Entanglement between modes (single-particle orbitals)

see e.g.: Legeza et al. PRC 92, 051303(R) (2015) in the framework of DMRG using Shell Model interactions;
Kruppa et al. J. Phys. G: Nucl. Part. Phys. 48 025107 (2021) two-nucleon systems in the Shell Model

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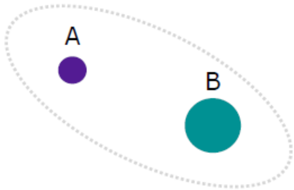
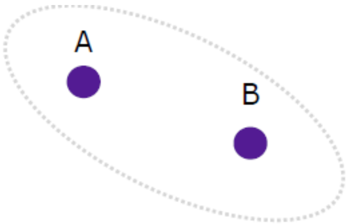
A Complication-Orbital Entanglement

Entanglement in systems with distinguishable particles:
Well understood – Hilbert Space has a tensor like structure



$$H_{tot} = H_A \otimes H_B \quad .$$

Entanglement in systems with indistinguishable particles:
Not well understood-under debate



$$\mathcal{H} = \mathcal{S}\left(\mathcal{H}_A \otimes \mathcal{H}_B\right) \quad (bosons) \qquad or \qquad \mathcal{H} = \mathcal{A}\left(\mathcal{H}_A \otimes \mathcal{H}_B\right) \quad (fermions)$$

Define entanglement between modes Rather then particles
(second quantization)

Calculating Orbital Entanglement

$$|\Psi\rangle = \sum_{\eta} \mathcal{A}_\eta |\phi_\eta\rangle$$

$$\rho^{(i)} = \begin{pmatrix} 1-\gamma_{ii} & 0 \\ 0 & \gamma_{ii} \end{pmatrix}$$

One Orbital Density Matrix

$$\gamma_{ii} = \langle\Psi|a_i^\dagger a_i|\Psi\rangle$$

Slater determinant

$$|\phi_\eta\rangle = \prod_{i\in\eta}^{A} a_i^\dagger|0\rangle$$

$$S_i^{(1)} = -Tr[\rho^{(i)}\ln\rho^{(i)}] = -\sum_{k=1}^{2}\omega_k^{(i)}\ln\omega_k^{(i)}$$

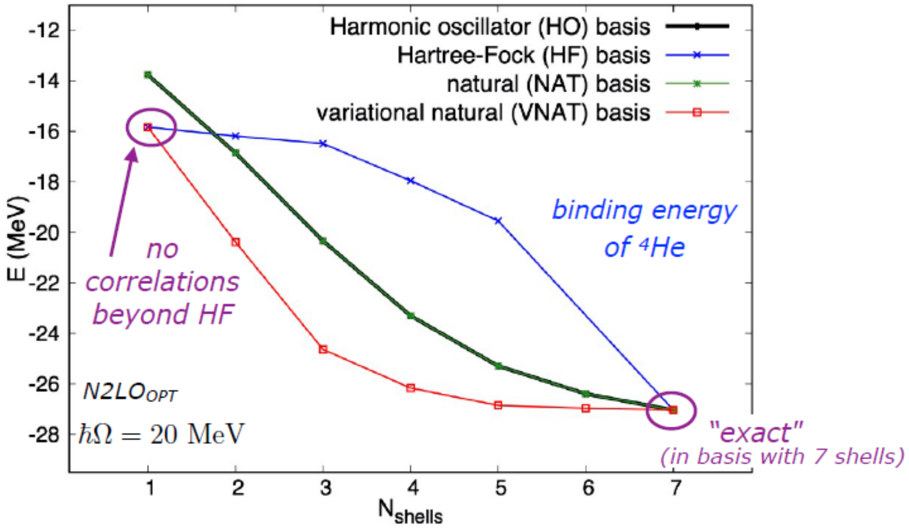
The ω_k are eignevalues of ρ_i

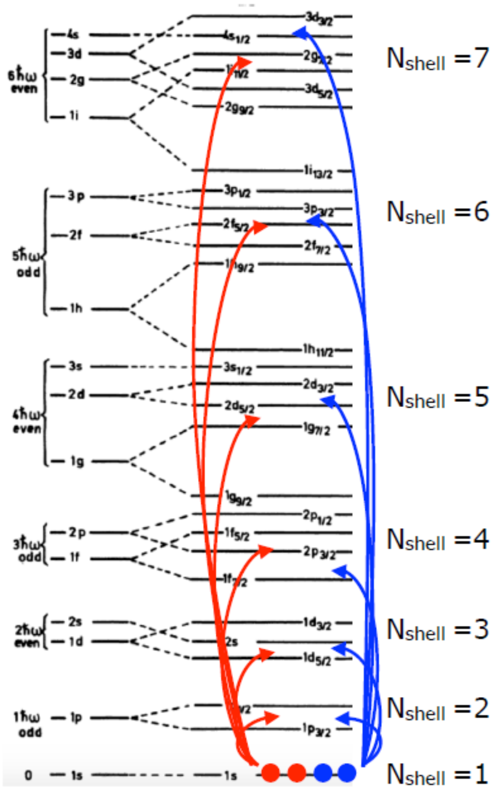
What has been Calculated for Nuclear structure

★ ***application to ^{4}He with a bare chiral interaction*** *(2-body force, provided by P. Navrátil)*

single-particle bases expanded on 7 HO major shells

full diagonalization in active space with $N_{shell} \leq 7$





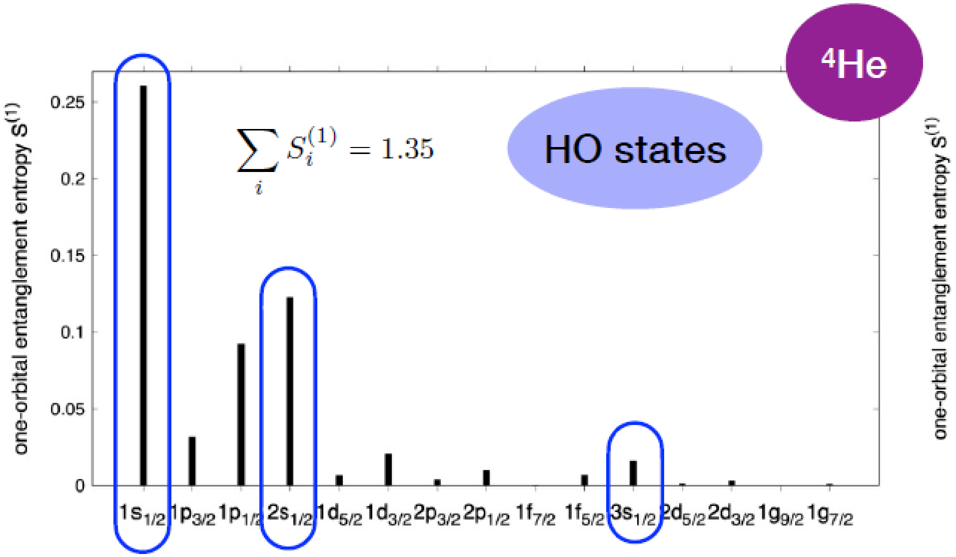
Here: mode entanglement in (very) light nuclei with chiral EFT interaction

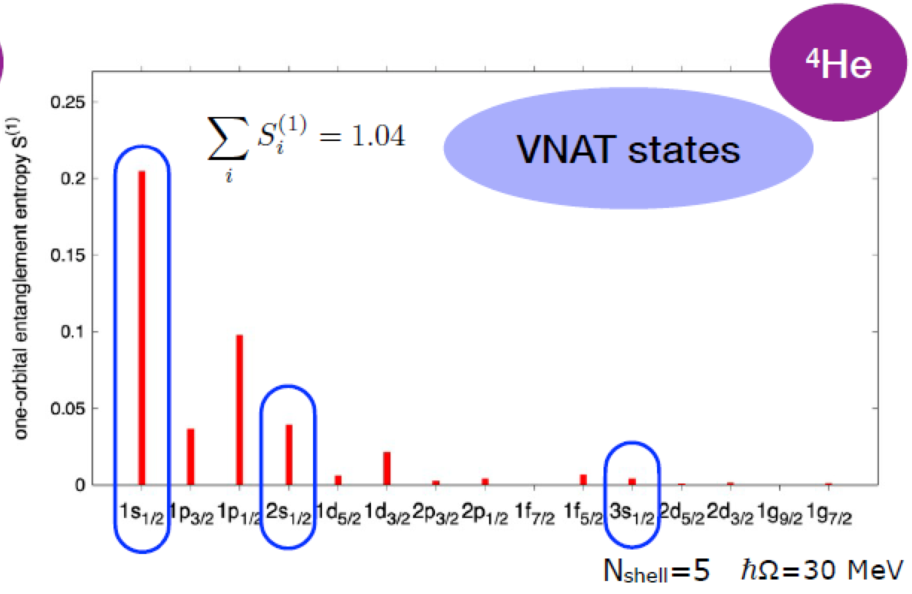
C. Robin, M. J. Savage, N. Pillet, PRC 103, 034325 (2021), arXiv:2007.09157 [nucl-th] (2020)

Single-Orbital Entanglement in ^{4}He

- Single-orbital Von Neumann entropy:

  = measure of entanglement of one orbital with the rest of the system

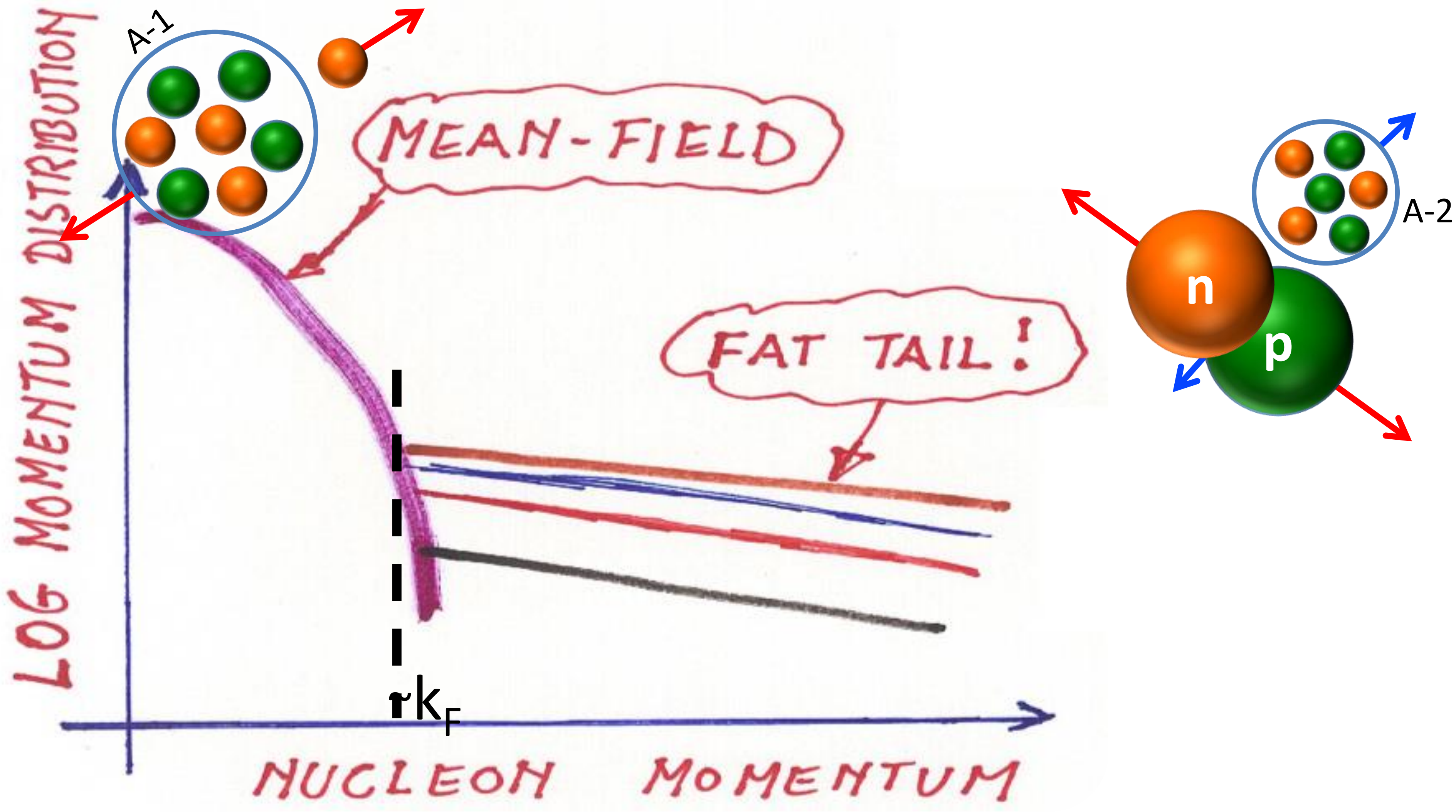




- *Entanglement of the s states are decreased: $(1s)_{VNAT}$ contains most important information*

$$(1s)_{VNAT} = a_1(1s)_{HO} + a_2(2s)_{HO} + a_3(3s)_{HO}\ldots$$

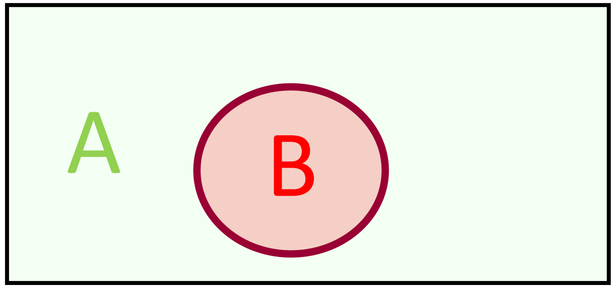
General Contact Formalism (GCF)



General Contact Formalism (GCF)

ansatz

$$\Psi \xrightarrow[r_{ij}\to 0]{} \varphi(\boldsymbol{r}_{ij}) A(\boldsymbol{R}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j})$$



Two Body Universal wave function
in terms of:
Relative coordinate $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$

A function of the A-2 remaining nucleons
also in terms of:
Center of mass coordinate $\boldsymbol{R}_{ij} = (\boldsymbol{r}_i + \boldsymbol{r}_j)/2$

The Contact

$$C_{pn} = N(A,Z)\langle A_{pn}^{\alpha_1} | A_{pn}^{\alpha_1}\rangle$$

$$\langle A|A\rangle = \int d^3R_{ij} \prod_{k\neq i,j} d^3r_k \; A^\dagger\left(\boldsymbol{R}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j}\right) A\left(\boldsymbol{R}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j}\right)$$

The contact traces over all of the degrees of freedom aside from the pair

Calculating the SRC Entanglement Entropy

- The SRC Entanglement entropy is the sum of the Entanglement Entropy of SRC pairs.
- Calculating the entanglement entropy of a single pair.
- Comparing results with the ^{4}He calculations.
- The Fermi Gas part.

SRC Entanglement Entropy is a sum of the Entanglement Entropy of Single SRC

Assumption: the total SRC entanglement entropy is the sum of the number of SRC pairs-
Meaning assuming SRC pairs are not entangled between themselves

$$S_A^{SRC} = \sum_i^N S_i^{SRC}$$

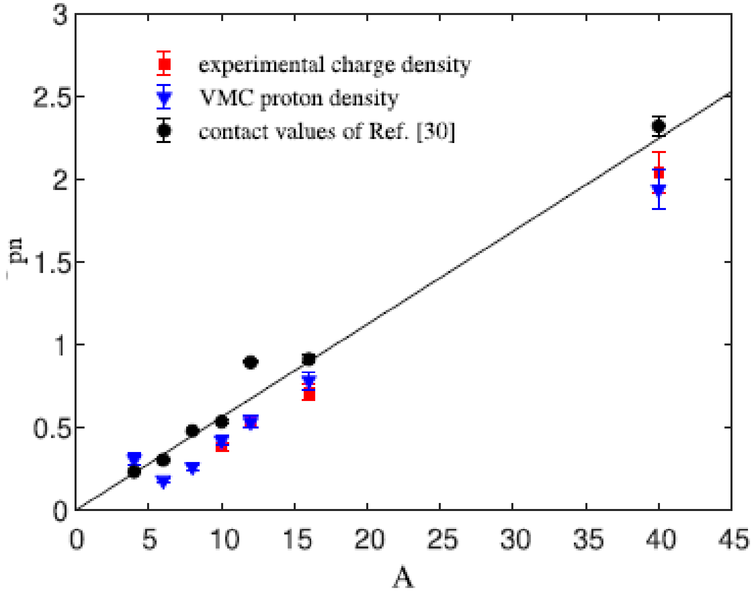
The probability for obtaining a single SRC pair is given by the normalized contact

$$c_{pn} \equiv \frac{C_{pn}}{(A/2)}$$

The Normalized Contact

The probability for obtaining a single SRC pair

$$c_{pn} \equiv \frac{C_{pn}}{(A/2)}$$



This normalization of the contact Gives the fraction of the one body momentum density above KF

Calculations for the single SRC entanglement entropy will be done with the normalized contact which is A independent

Ronen Weiss [a,*], Axel Schmidt [b], Gerald A. Miller [c], Nir Barnea [a] Physics Letters B 790 (2019) 484–489

Calculating the single SRC Entanglement Entropy

$$\rho^{(i)} = \begin{pmatrix} 1-\gamma_{ii} & 0 \\ 0 & \gamma_{ii} \end{pmatrix} \longrightarrow$$

$$S_i^{(1)} = -Tr[\rho^{(i)} \ln \rho^{(i)}] = -\sum_{k=1}^{2} \omega_k^{(i)} \ln \omega_k^{(i)}$$

One Orbital Density Matrix

$$\gamma_{ii} = \langle \Psi | a_i^\dagger a_i | \Psi \rangle$$

SRC

The probability an SRC is occupied

$$\gamma_{SRC} = c_{pn}$$

$$\rho^{(\alpha_1)} = \begin{pmatrix} 1-\gamma_{SRC} & 0 \\ 0 & \gamma_{SRC} \end{pmatrix} \longrightarrow$$

$$S_{pn}^{SRC} = -\left[c_{pn} \ln \left(\frac{c_{pn}}{1-c_{pn}} \right) + \ln(1-c_{pn}) \right]$$

Calculating the SRC Entanglement Entropy

$$S_A^{SRC} = -\frac{A}{2}\left[c_{pn}\ln\left(\frac{c_{pn}}{1-c_{pn}}\right) + \ln\left(1-c_{pn}\right)\right]$$

The SRC Entanglement Entropy is extensive ~A

E. Pazy, Orbital Entanglement Entropy of Short Range Correlated Pairs in Nuclear Structure arXiv:2206.10702

Comparing to Previous Results for ^{4}He

$$S_{tot}^{(1)} = \sum_i S_i^{(1)}$$

N_{tot}	HO	HF	NAT	VNAT
2 shells	0.596	0.270	0.596	0.441
3 shells	1.143	0.487	0.929	0.746
4 shells	1.065	0.686	0.928	1.063
5 shells	1.348	2.327	1.036	1.042
6 shells	1.264	3.434	0.972	0.963
7 shells	1.217	1.069	1.006	1.006

$$S_A^{SRC} = -\frac{A}{2}\left[c_{pn}\ln\left(\frac{c_{pn}}{1-c_{pn}}\right) + \ln(1-c_{pn})\right]$$

$$S_A^{SRC} = 0.72$$

$$c_{pn} = 0.12$$

$$S_A^{SRC} = 0.84$$

$$c_{pn}^{exp} = 0.15$$

- Proton-Proton and Neutron –Neutron pairs were not considered.
- Two orbital entanglement was not considered.

Quite a good agreement with previous results

E. Pazy, Orbital Entanglement Entropy of Short Range Correlated Pairs in Nuclear Structure arXiv:2206.10702

What has been Calculated for Nuclear structure

Entropy, single-particle occupation probabilities, and short-range correlations

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(Dated: June 9, 2022)

Both theoretical and experimental studies have shown that the fermion momentum distribution has a generic behavior $n(k) = C/k^4$ at momenta larger than the Fermi momentum, due to their short-range interactions, with approximately 20% of the particles having momenta larger than the Fermi momentum. It is shown here that short-range correlations, which induce high-momentum tails of the single-particle occupation probabilities, increase the entropy of fermionic systems, which in its turn will affect the dynamics of many reactions, such as heavy-ion collisions and nuclear fission.

$$S = -g\int \frac{d^3k}{(2\pi)^3} n(k) \ln n(k) - g\int \frac{d^3k}{(2\pi)^3}[1-n(k)]\ln[1-n(k)], \qquad (5)$$

The Entropy in Terms of the Canonical momentum occupation function

The Entropy in Terms of the Canonical momentum occupation function

$$S = -g \int \frac{d^3k}{(2\pi)^3} n(k) \ln n(k) - g \int \frac{d^3k}{(2\pi)^3} [1 - n(k)] \ln[1 - n(k)], \qquad (5)$$

$$n(k) = \eta(k_0) \begin{cases} n_{\mathrm{mf}}(k), & \text{if} \quad k \leq k_0 \\ n_{\mathrm{mf}}(k_0) k_0^4 \frac{1}{k^4}, & \text{if} \quad k_0 < k < \Lambda \end{cases}, \qquad (9)$$

$$n(k) = C/k^4$$

where

$$C(k_0) = \eta(k_0) n_{\mathrm{mf}}(k_0) k_0^4 \qquad (10)$$

Reconciling the two views: canonical momentum occupation and GCF

$$S = -g\int \frac{d^3k}{(2\pi)^3} n(k)\ln n(k) - g\int \frac{d^3k}{(2\pi)^3}[1-n(k)]\ln[1-n(k)], \qquad (5)$$

$$n(k) = C/k^4$$

$$S = -\frac{g}{2\pi^2}\int_{k_0}^{\Lambda}\left[\frac{C}{k^2}\ln\left(\frac{\frac{C}{k^4}}{1-\frac{C}{k^4}}\right) + k^2\ln\left(1-\frac{C}{k^4}\right)\right]$$

Estimating the integral as lower limit time K_0

$$S \approx -\frac{g}{2\pi^2}\left[\frac{C}{k_0}\ln\left(\frac{\frac{C}{{k_0}^4}}{1-\frac{C}{{k_0}^4}}\right) + {k_0}^3\ln\left(1-\frac{C}{{k_0}^4}\right)\right]$$

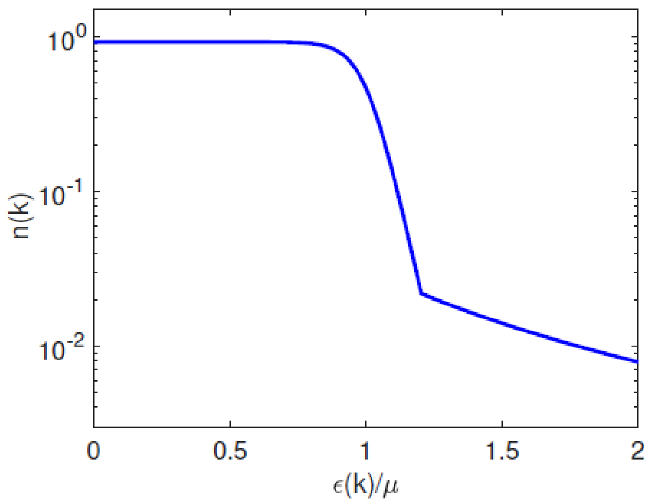


FIG. 5. The generic dependence of the canonical momentum occupation probability $n(k)$ versus the kinetic energy $\epsilon(k)$ after taking into the account the role of the short-range correlations, a result similar to the behavior established for finite systems in Ref. [2].

Reconciling the two views

$$S \approx -\frac{g}{2\pi^2}\left[\frac{C}{k_0}\ln\left(\frac{\frac{C}{{k_0}^4}}{1-\frac{C}{{k_0}^4}}\right)+{k_0}^3\ln\left(1-\frac{C}{{k_0}^4}\right)\right]$$

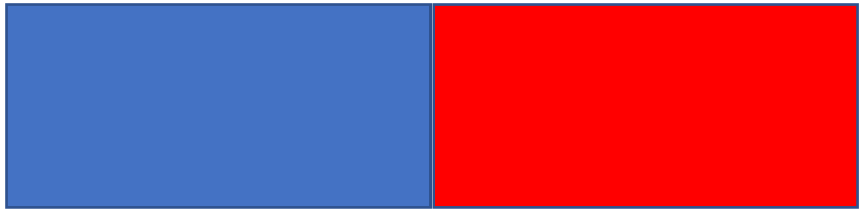
$$C/{k_F}^4 \sim C/k_F A \equiv c_{pn}$$

$$S \approx -\frac{g{k_F}^3}{2\pi^2}\left[c_{pn}\ln\left(\frac{c_{pn}}{1-c_{pn}}\right)+\ln\left(1-c_{pn}\right)\right]$$

$$g{k_F}^3/6\pi^2 \approx A$$

Comparing the SRC with the Fermi Sea Entanglement Entropy

$$S_{SRC|FS} = -Tr\left(\rho_{FS}\ln\rho_{FS}\right) = -Tr\left(\rho_{SRC}\ln\rho_{SRC}\right)$$



Calculating the Entanglement Entropy for the Fermi Sea

General Formula for the Entanglement Entropy of a Fermi Sea

$$S^{FS} = \frac{L^{d-1}}{(2\pi)^{d-1}} \frac{\log L}{12} \int\int |n_x \cdot n_k| dA_x dA_k$$

Nuclear structure Calculation

$$S_A^{FS} = (1 - c_{pn}) \frac{\log L}{12} \tilde{u}_s A^{\frac{2}{3}} = (1 - c_{pn}) \frac{\log A}{36} \tilde{u}_s A^{\frac{2}{3}}$$

The naïve Fermi sea calculation of the Entanglement Entropy satisfies an area law. Does not match SRC Entanglement Entropy!

Summary

- A general expression was obtained for the SRC Entanglement Entropy.
- The SRC Entanglement Entropy was found to be extensive.
- The SRC entanglement entropy seems to fit previous ^4He calculations.
- The naïve Fermi Gas Entanglement entropy approximation does not seem to work.

Thank you!