Nuclear Orbital Entanglement Entropy of Short Range Correlations

4-th International Workshop on Quantitative Challenges in Short-Range Correlations and the EMC Effect Research

CEA Paris-Saclay
February 1st

Ehoud Pazy
NRCN

Outline-Introduction

Entanglement

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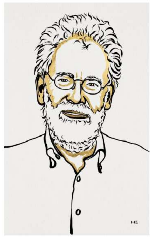

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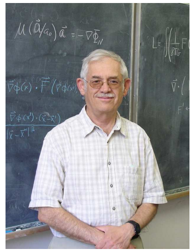
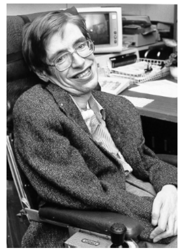
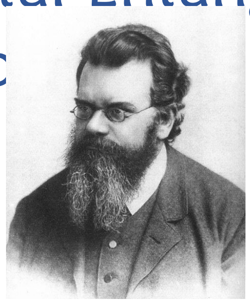
Entanglement entropy
Area law





Orbital Entanglement
entrc



Short Range
Correlated (SRC) pairs

Outline-Introduction

A Secret Ingredient
The Generalized Contact Formalism (GCF)

Calculating Entanglement Entropy for SRC:

- Calculating the entanglement entropy of a single SRC pair in term of the contact.
- Summing up the Entanglement Entropy of SRC pairs.
- Comparing results with the ^{4}He calculations.

The Main Questions

How to calculate the entanglement entropy of the SRC?
Does it obey an Area Law?
Is most of the entanglement entropy in SRC?

Entanglement

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

The Nobel Prize in Physics 2022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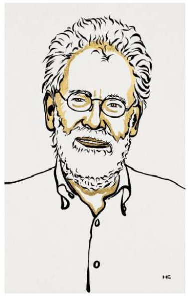
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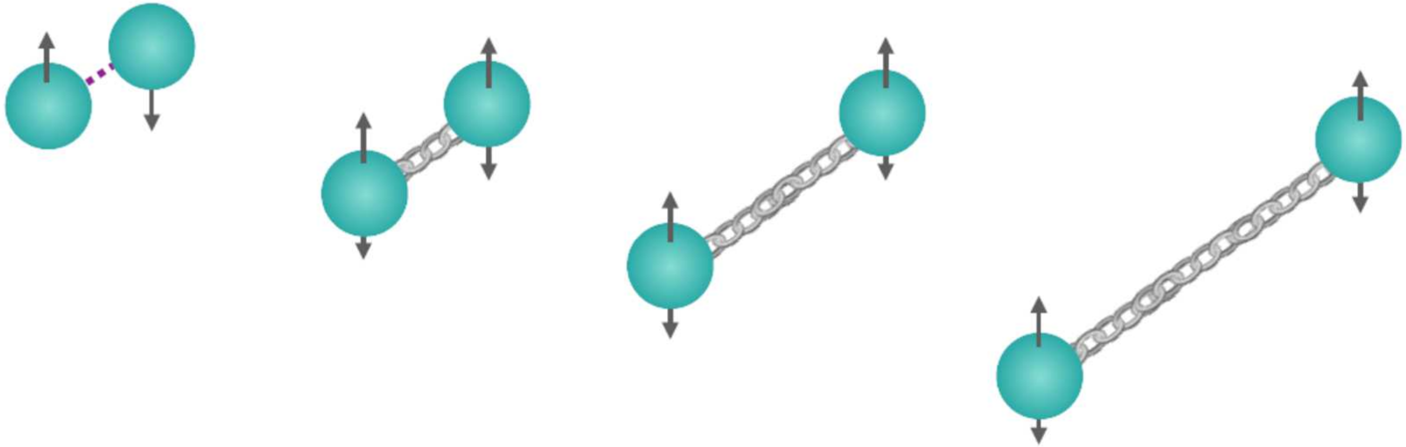
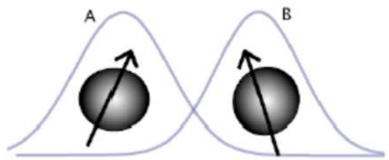
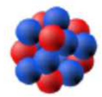


Entanglement at short distance, when particles have overlapping wave functions:



ex: nucleons in the nucleus



Caroline Robin

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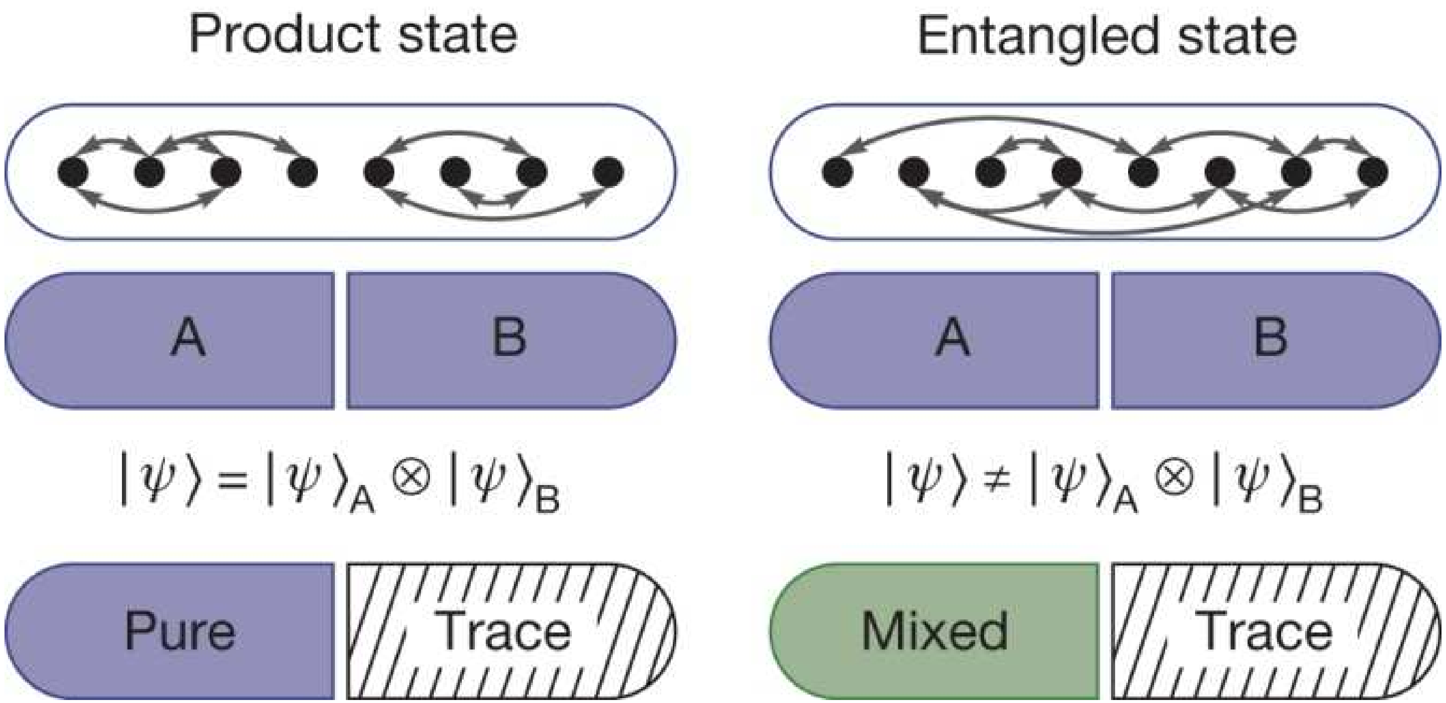
Entanglement Entropy

Arises due to tracing out some part of the system

- In contrast to thermal states this entropy does not originate from a lack of knowledge about the microstate of the system.
- In quantum mechanics positive entropies may arise even without an objective lack of information.
- Even at zero temperature we will encounter a non-zero entropy!
- This entropy arises because of a very fundamental property of quantum mechanics: Entanglement

J. Eisert, M. Cramer, and M.B. Plenio, **Reviews of Modern Physics (2010)**

Entanglement Entropy: Product verses Entangled



S=0

S>0

R Islam *et al. Nature* **528,** 78 (2015) doi:10.1038/nature15750

Definition of Entanglement Entropy

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

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

We define the reduced density matrix ρ_A for A by

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

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

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

Simple example of Entanglement Entropy

$$|\Psi\rangle = \sum_{ab} \Psi_{ab}|a\rangle \otimes |b\rangle \rightarrow \underline{\Psi} = \begin{bmatrix} \Psi_{\uparrow\uparrow} & \Psi_{\uparrow\downarrow} \\ \Psi_{\downarrow\uparrow} & \Psi_{\downarrow\downarrow} \end{bmatrix}$$

where the basis vectors $|a\rangle$ and $|b\rangle$ are either $|\uparrow\rangle$ or $|\downarrow\rangle$

$$S_{pn} = -\sum_i \gamma_i^2 \ln(\gamma_i^2)$$

Non Entangled case

$$|\Psi\rangle = |\uparrow\downarrow\rangle \rightarrow \underline{\Psi} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \qquad \underline{\rho}_1 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad S_{12} = S(\rho_1) = -(1\ln(1) + 0\ln(0)) = 0.$$

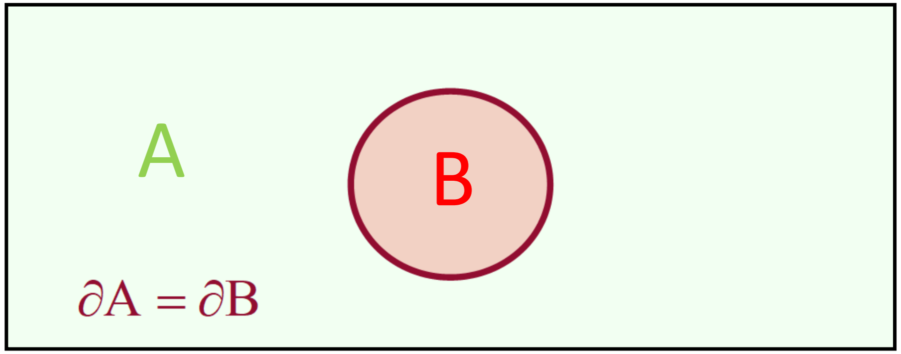
Entangled case

$$|\Psi'\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \underline{\Psi}' = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad \underline{\rho}' = \underline{\Psi}' * \underline{\Psi}'^{\dagger} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Master Thesis, Oliver Gorton , 2018

$$S_{12} = S(\rho_1) = -(\frac{1}{2}\ln(\frac{1}{2}) + \frac{1}{2}\ln(\frac{1}{2})) = \ln 2$$

Entangled Entropy Area Law



"At first sight one might be tempted to think that the entropy of a distinguished region B, will always possess an extensive character. Such a behavior is referred to as a volume scaling and is observed for thermal states.
Intriguingly, for typical ground states, however, this is not at all what one encounters:
Instead, one typically finds an area law, or an area law with a small (often logarithmic) correction: This means that if one distinguishes a region, the scaling of the entropy is merely linear in the boundary area of the region."

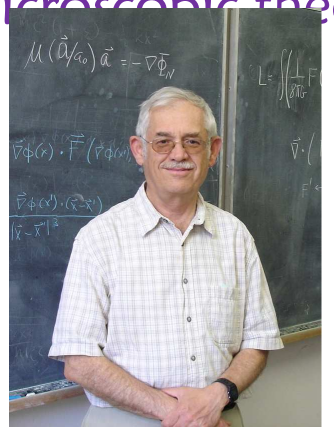
J. Eisert, M. Cramer, and M.B. Plenio, **Reviews of Modern Physics (2010)**

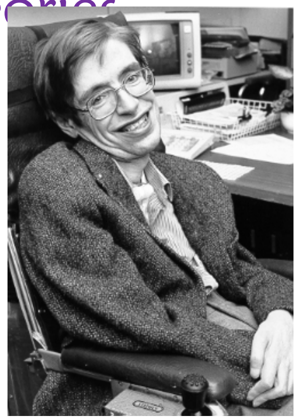
The Holographic Principle and Black Hole Entropy

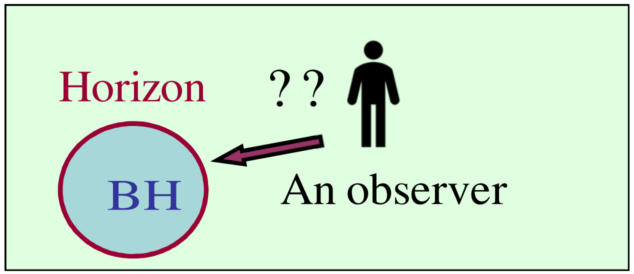
“It has been suggested that the area law of the geometric entropy for a discrete version of a massless free scalar field— then numerically found for an imaginary sphere in a radial symmetry—could be related to the physics of black holes, in particular the Bekenstein-Hawking entropy of a black hole which is proportional to its boundary surface.

It has been noted that 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 ∂A ~ the event horizon

J. Eisert, M. Cramer, and M.B. Plenio, **Reviews of Modern Physics** (2010)

Why is the Nuclear Structure Entanglement Entropy Important?

- Computational- efficiency.
- Physics- dynamics of reactions:

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?

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

$$|01101000...\rangle|10010100...\rangle$$

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

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!)

Why is Entanglement Entropy Important for Nuclear Structure?

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

Aurel Bulgac[1,*]

[1] *Department of Physics, University of Washington, Seattle, Washington 98195–1560, USA*

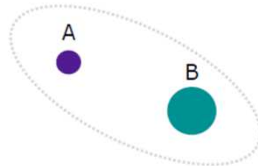
(Dated: June 9, 2022)

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.

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.

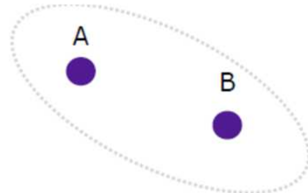
A Complication Orbital Entanglement

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



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

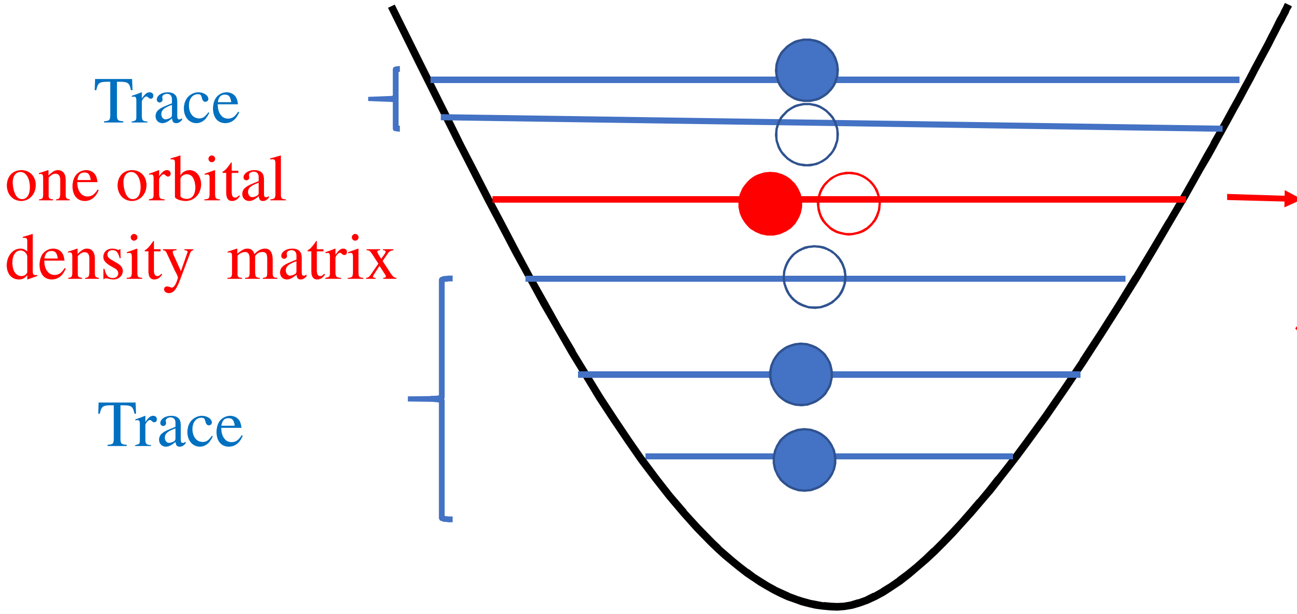
Entanglement in systems with indistinguishable particles:
Not well understood-under debate



$\mathcal{H} = \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$ *(bosons)* *or* $\mathcal{H} = \mathcal{A}(\mathcal{H}_A \otimes \mathcal{H}_B)$ *(fermions)*

Define entanglement between modes Rather than particles (second quantization)

Orbital Entanglement



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

von Neumann entropy

Calculating Orbital Entanglement

$$|\Psi\rangle = \sum_{\eta} A_\eta |\phi_\eta\rangle \longrightarrow \rho^{(i)} = \begin{pmatrix} 1-\gamma_{ii} & 0 \\ 0 & \gamma_{ii} \end{pmatrix}$$

One Orbital Density Matrix

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

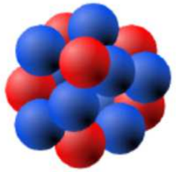
Slater determinant

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

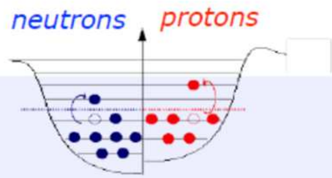
$$S_i^{(1)} = -Tr[\rho^{(i)} \ln \rho^{(i)}] = -\sum_{k=1}^{2} \omega_k^{(i)} \ln \omega_k^{(i)}$$

The ω_k are eignevalues of ρ_i

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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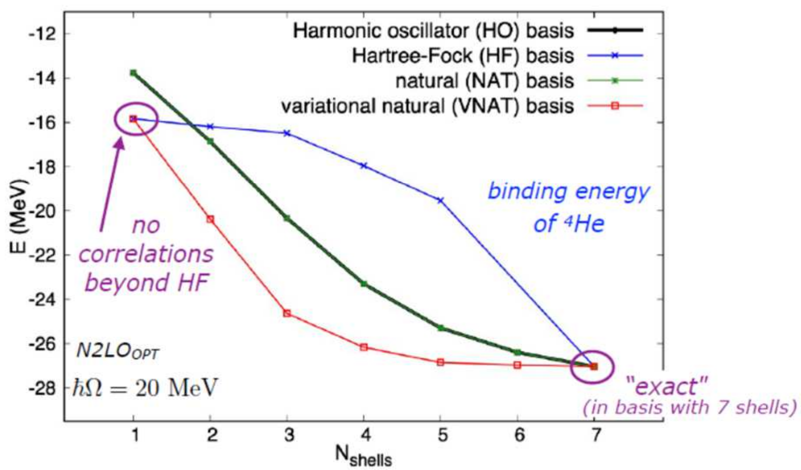
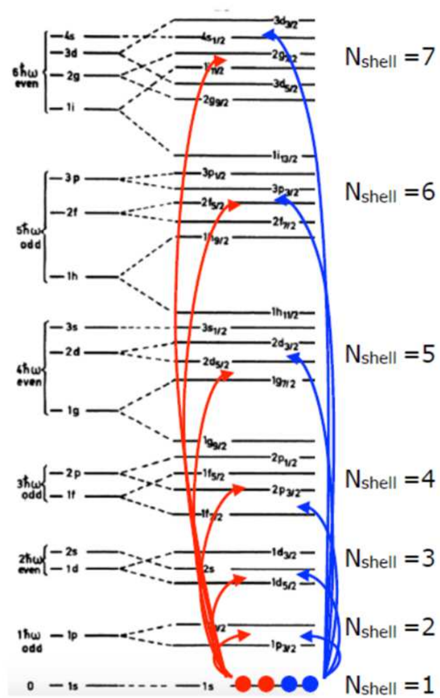
What has been Calculated for Nuclear Structure?

★ ***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 $N_{shell} \leq 7$





Limited to light nuclei

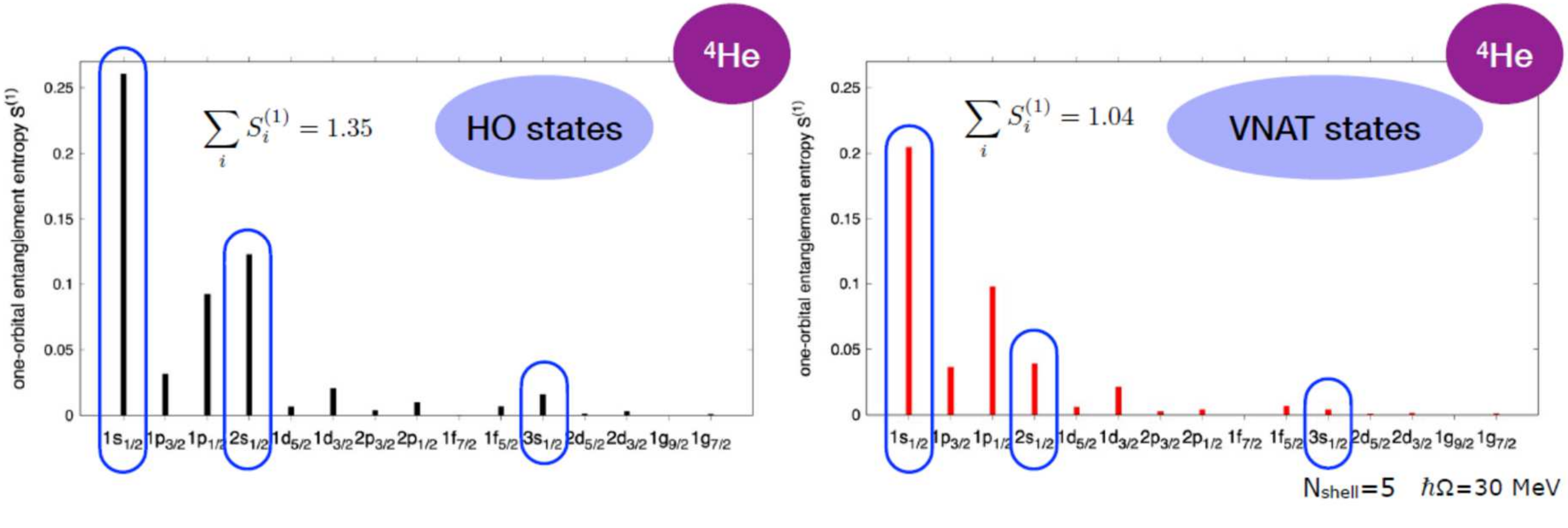
Here: mode entanglement in (very) light nuclei with chiral EFT interaction

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

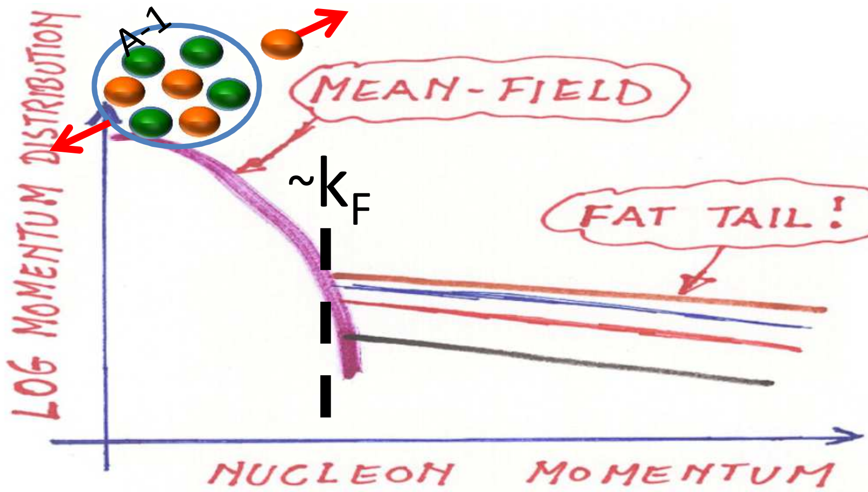


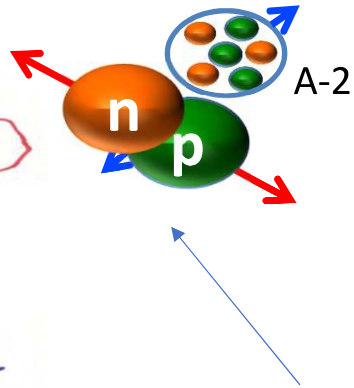
- *Entanglement of the s states are decreased: $(1s)_{VNAT}$ contains most important information*

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

Limited to light nuclei

A Different Approach Based on the General Contact Formalism (GCF)





A universal two particle state

Pappalardo Fellowship
20th Anniversary Colloquium, April 28th (2022)

- Universal in some sense.
- Simple to calculate.

A Different Approach Based on the General Contact Formalism (GCF)

The two particle state is Universal

- It can be viewed as a further “orbital” particles can occupy.
- It’s “occupancy” is given by the contact.
- The entanglement of the SRC can be given as a simple formula based on the contact.

General Contact Formalism (GCF)

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

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

SRC Momentum Distribution in GCF

Given the following normalization $$\int_{k_F}^{\infty} d^3q|\varphi_{ab}^{\alpha}(q)|^2 = 1$$

The Contact can be viewed as the probability for obtaining a SRC in the nucleus /
The occupation of the universal two state "orbital"

$$F_{pn}(\mathbf{q}) = \rho_{pn}^{\alpha_1}(\mathbf{q})C_{pn}$$

$$\rho_{pn}^{\alpha_1}(\mathbf{q}) = |\varphi_{pn}^{\alpha_1}(\mathbf{q})|^2$$

Calculating the SRC Entanglement Entropy

- The Universal two-particle wave function can be viewed as a further “orbital”.
- The occupation probability of this orbital is given by the contact.

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

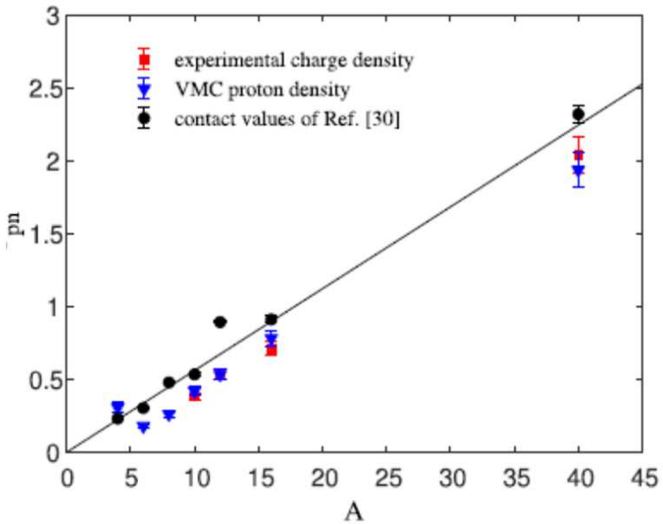
$$C_{pn} = N(A,Z)\langle A_{pn}^{\alpha_1} | A_{pn}^{\alpha_1} \rangle \quad N(A, Z = A/2) = \frac{A}{2} \frac{\int_{k_F}^{\infty} n(k)dk}{\int_0^{\infty} n(k)dk} = C_{pn}/(A/2)$$

$$c_{pn} \equiv \frac{C_{pn}}{(A/2)} \qquad \gamma_{SRC} = c_{pn}$$

The Normalized Contact

The probability for obtaining a single SRC pair

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



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 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

$$\int_{k_F}^{\infty} d^3q |\varphi_{ab}^{\alpha}(q)|^2 = 1$$

Sum over momentum

$$\rho^{(\alpha_1)} = \sum_{\phi_{\eta'}} \langle \phi_{\eta'} | \langle \tilde{\varphi}_q^{\alpha_1} | \Psi \rangle \langle \Psi | \tilde{\varphi}_q^{\alpha_1} \rangle | \phi_{\eta'} \rangle$$

$$\gamma^{\alpha_1} = \int_{k_F}^{\infty} d^3q \rho_{pn}^{\alpha_1}(q) c_{pn} = c_{pn} \int_{k_F}^{\infty} d^3q \rho_{pn}^{\alpha_1}(q) = c_{pn}$$

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

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

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

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

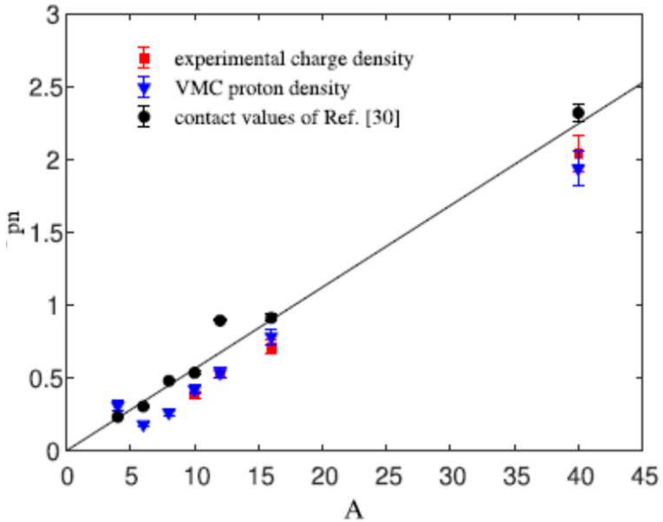
The probability for obtaining a single SRC pair is given by the normalized contact

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

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

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

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

One Orbital Density Matrix

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

SRC

The probability an SRC is occupied

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

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

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

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.

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

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

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where

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

ssociating the reduced contact with $c_{pn} = C/k_F{}^4$ one obtains

$$S \approx -3A\left[c_{pn}\ln\left(\frac{c_{pn}}{1-c_{pn}}\right) + \ln(1-c_{pn})\right]$$

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.

Thank You for your Attention and Bonne Appetit