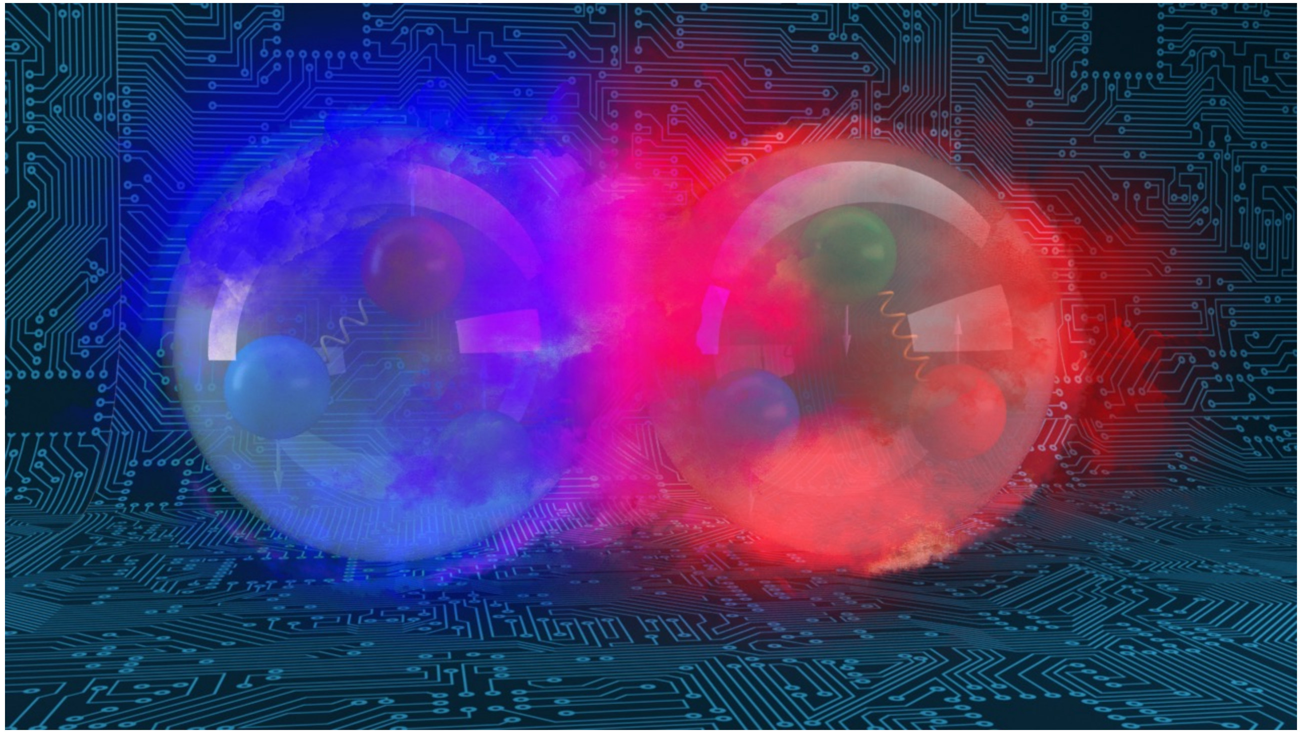
Entanglement in nuclear models and matter



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Quantum Computing for Many-Body problems (QCMB): atomic nuclei, neutrinos, and other strongly correlated Fermi systems
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QUANTUM SCIENCE CENTER

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NUCLEI
Nuclear Computational Low-Energy Initiative

Entanglement in nuclei

Correlations, wave-function complexity, entanglement, …

Correlations: quantified by correlation energy
- Shina Tan's contact and its generalizations [Weiss, Bazak, Barnea 2015]
- RG approaches: resolution scale and short-range correlations [Tropiano, Bogner, Furnstahl 2021]
- Methods: coupled-cluster theory, QRPA approach, VMC

Wave function complexity: quantified by statistics
- Random matrix theory; level repulsion; Porter-Thomas distributions
- Spectral fluctuations and chaos in nuclear spectra [Bohigas, Haq, Panday 1985; Zelevinsky, Brown, Frazier & Horoi 1996; TP & Weidenmüller 2007; Mitchell, Richter, Weidenmüller 2010; …]

Entanglement: quantify by entanglement entropies
- Density matrix renormalization group [White 1992], adopted in nuclear physics [Dukelsky & Dussel 1999; Dukelsky & Pittel 2001; Dukelsky, Pittel, Dimitrova, Stoitsov 2002; TP & Dean 2005; Rotureau et al 2007; Legeza, Veis, Poves, Dukelsky 2015; …] see Kevin Fossez' page https://kevinfossez.github.io/misc/DMRG/
- Entanglement in nuclear forces and nuclei: Beane, Kaplan, Klco, Savage 2019; Robin, Savage, Pillet 2021; Kruppa et al 2022; Tichai et al 2022; Faba, Martin, Robledo 2021; …

Entanglement between two regions A and B

Hilbert space is a product $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$

Density matrix of ground state $\rho = |\Phi\rangle\langle\Phi|$

Reduced density matrix $\rho_A = \mathrm{Tr}_B\, \rho$

Réyni (1961) entropies $$S_\alpha = \frac{1}{1-\alpha} \ln \mathrm{Tr}\, \rho_A^\alpha$$

Von Neumann (1932) entropy $$S_1 = \lim_{\alpha\to 1} S_\alpha = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

Key question: How do entanglement entropies scale with the size of the region A?

Entanglement between two regions A and B

Two main results for free fermions: Gioev & Klich, Phys. Rev. Lett. 96, 100503 (2006)

1. Area law (with log corrections) in d dimensions for region A of linear size L.

$$S_1 \sim L^{d-1} \log L$$

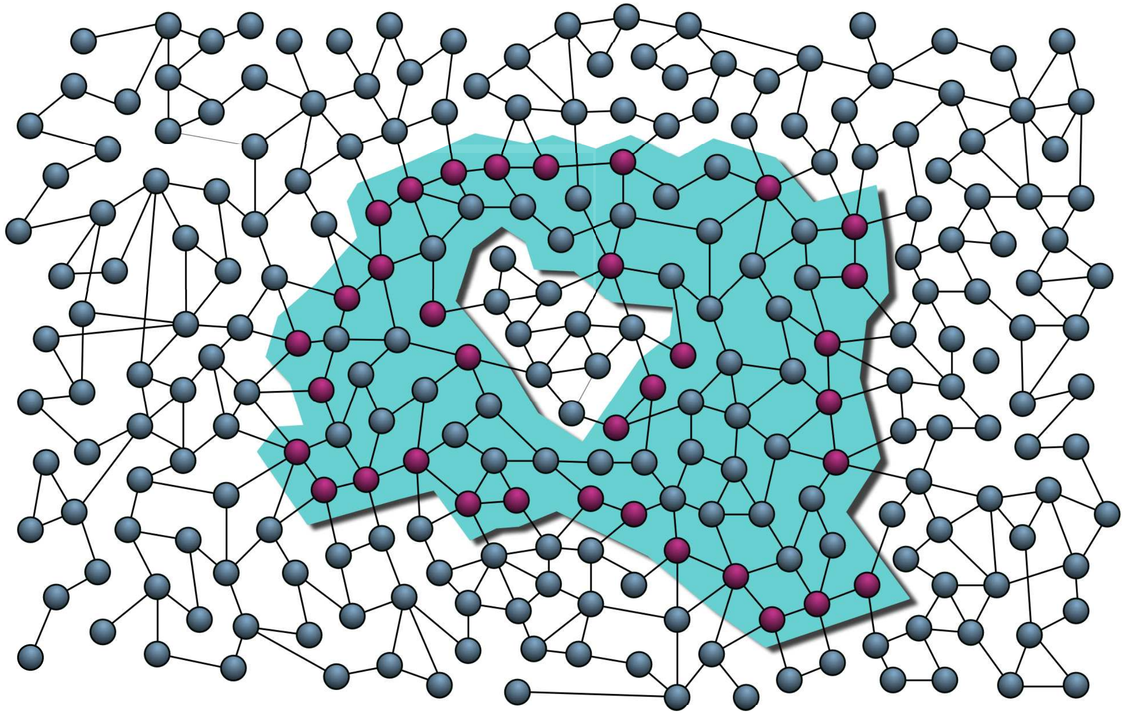
2. Particle number fluctuation in region A sets bounds on entropy

$$4(\Delta N)^2 \leq S_1 \leq \mathcal{O}(\log L)(\Delta N)^2$$

Extensions of these results: to Reyni entropies: Barthel, Dusuel, Vidal, Phys. Rev. Lett. 97, 220402 (2006); to an exactly solvable interacting system: Plenio, Eisert, Dreissig, and M. Cramer, Phys. Rev. Lett. 94, 060503 (2005); conditions for area laws: Masanes, Phys. Rev. A 80, 052104 (2009); …

Masanes (2009): Area law if " (i) the state has sufficient decay of correlations and (ii) the number of eigenstates with vanishing energy density is not exponential in the volume."

Expect area laws in lattice systems with local interactions



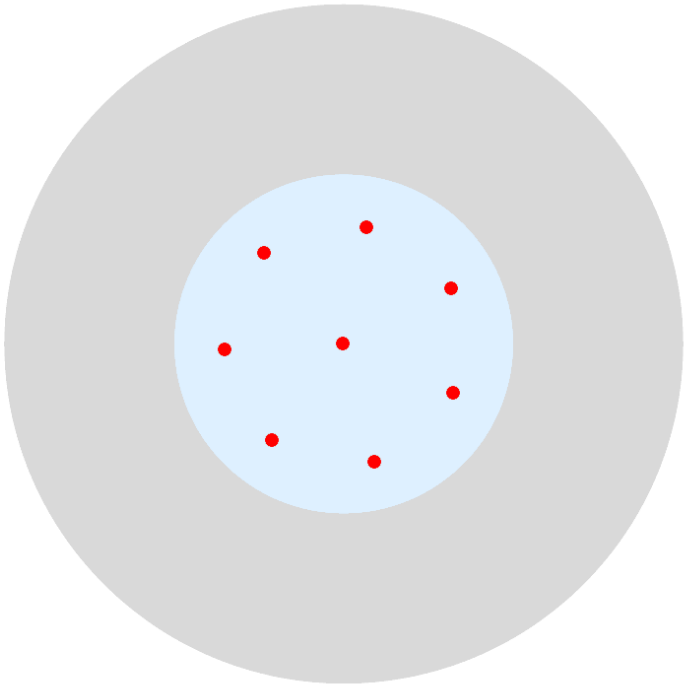
Eisert, Cramer, Plenio, Rev. Mod. Phys. 82, 277–306 (2010)
Lattice systems with local interactions intuitively fulfill area laws.

Masanes (2009): Area law if “ (i) the state has sufficient decay of correlations and (ii) the number of eigenstates with vanishing energy density is not exponential in the volume.”

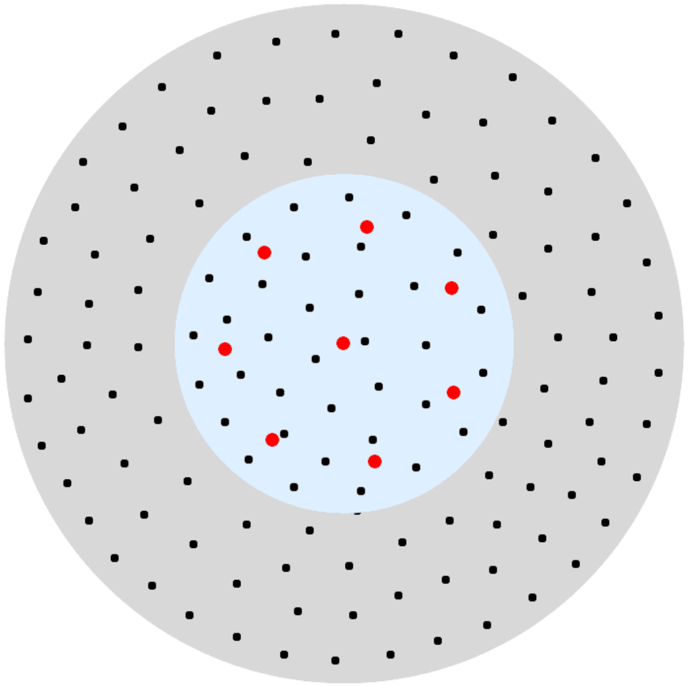
Expect volume law in nuclei

1. Perform HF calculation
2. Apply unitary transformations in particle and hole spaces to get localized basis states
3. Entanglement is between hole and particle space

Hole space: Localized occupied HF basis functions (red points) inside nucleus (blue); distance of points $\sim k_F^{-1}$.



Particle space: Localized unoccupied HF basis functions (black points); distance of points $\sim \Lambda^{-1}$.



We expect a volume law for nuclei as the cutoff and Fermi momentum approximately fulfill $\Lambda \gg k_F$

Analytical results for interacting systems

Reference state (hole state)

$$|\Phi_0\rangle = \prod_{i=1}^{N} \hat{a}_i^\dagger |0\rangle$$

Coupled-cluster theory

$$|\Psi_{\rm CC}\rangle = e^{\hat{T}}|\Phi_0\rangle \approx \left(1+\hat{T}_2\right)|\Phi_0\rangle \;= |\Phi_0\rangle + \frac{1}{4}\sum_{abij} t_{ij}^{ab}|\Phi_{ij}^{ab}\rangle$$

Rényi entropy

$$S_\alpha \approx \frac{t^{2\alpha} - \alpha t^2}{1-\alpha} + \mathcal{O}(t^4) \qquad t^2 \equiv \frac{1}{4}\sum_{i_1 i_2 a_1 a_2} t_{i_1 i_2}^{a_1 a_2} t_{i_1 i_2}^{a_1 a_2}$$

Rényi entropy vs. number fluctuation

$$\mathrm{S}_\alpha = \frac{\alpha}{4(\alpha-1)}\,\mathrm{Var}(N_H) + \mathcal{O}(t^4) \qquad N_H \equiv \sum_i \hat{a}_i^\dagger \hat{a}_i$$

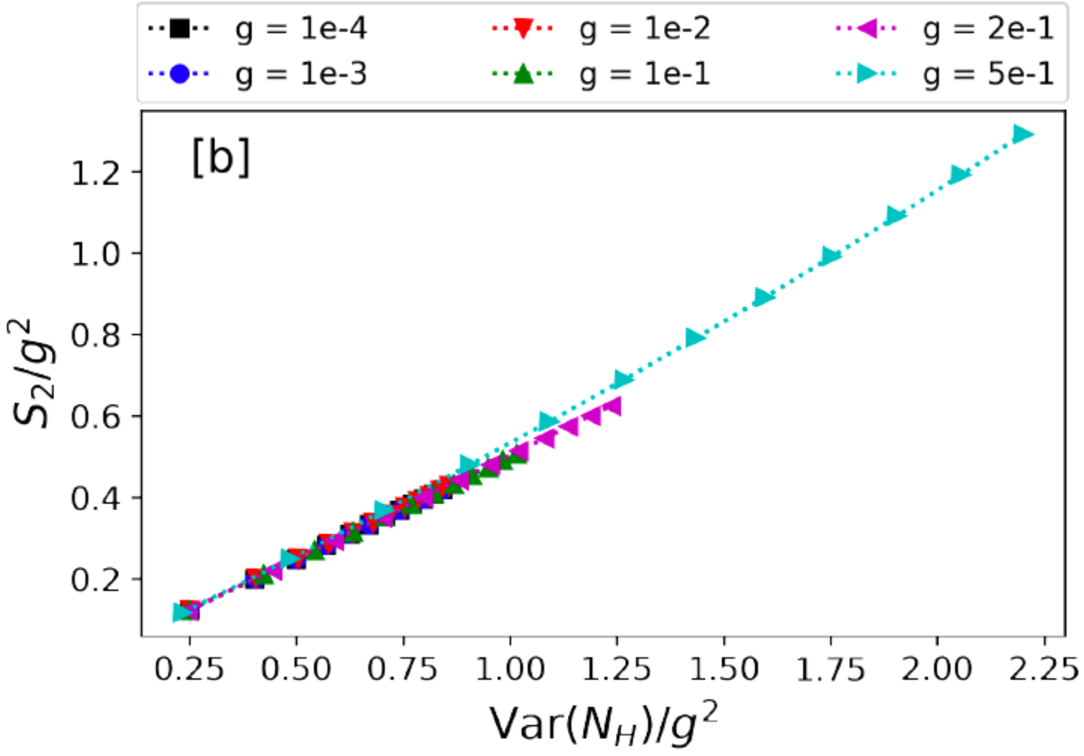
Caveat: For $\alpha \to 1$ need $t^2 < \;(\alpha-1)^{\frac{1}{\alpha-1}}$.

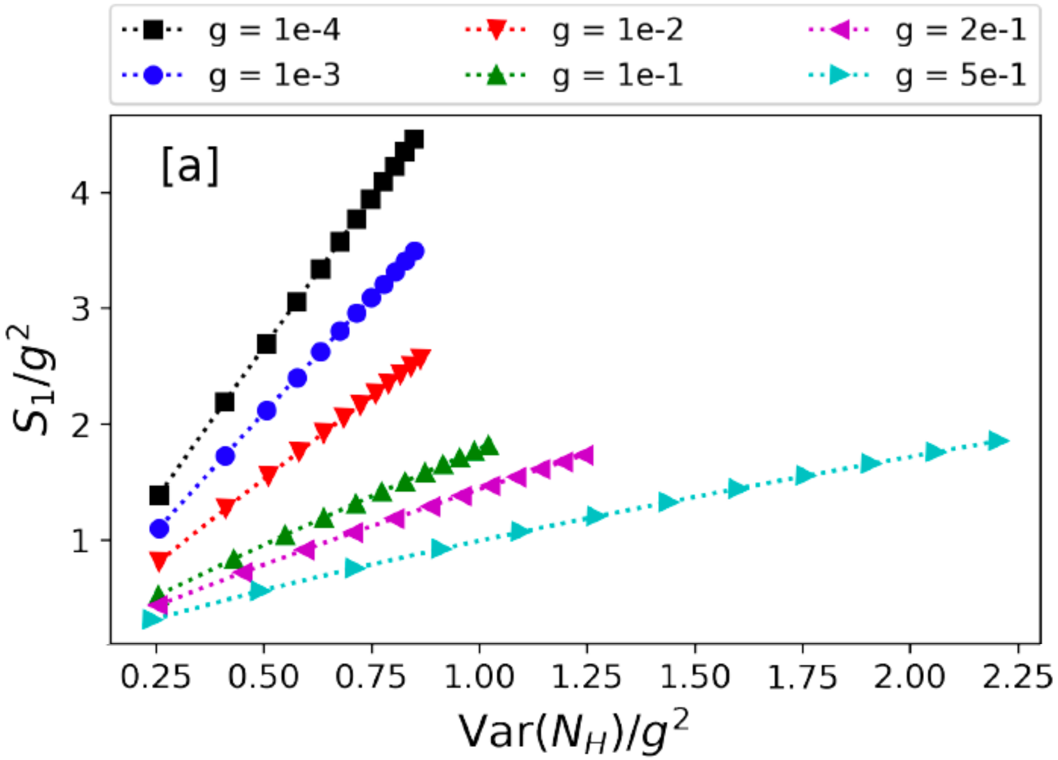
Open: Would like to understand how t^2depends on number of hole states

[Chenyi Gu, TP et al, in prep]

Numerical results for pairing model

$$\hat{H} = \delta \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma} - \frac{1}{2} g \sum_{pq} a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+}$$



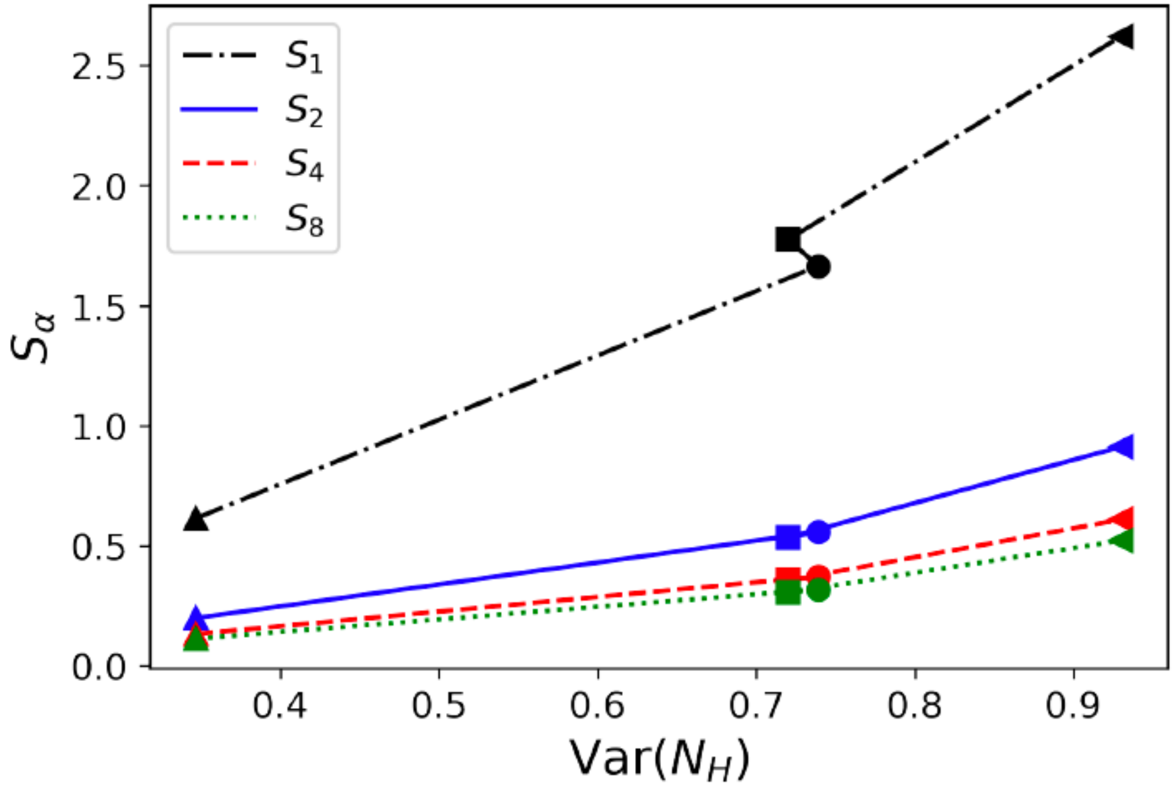


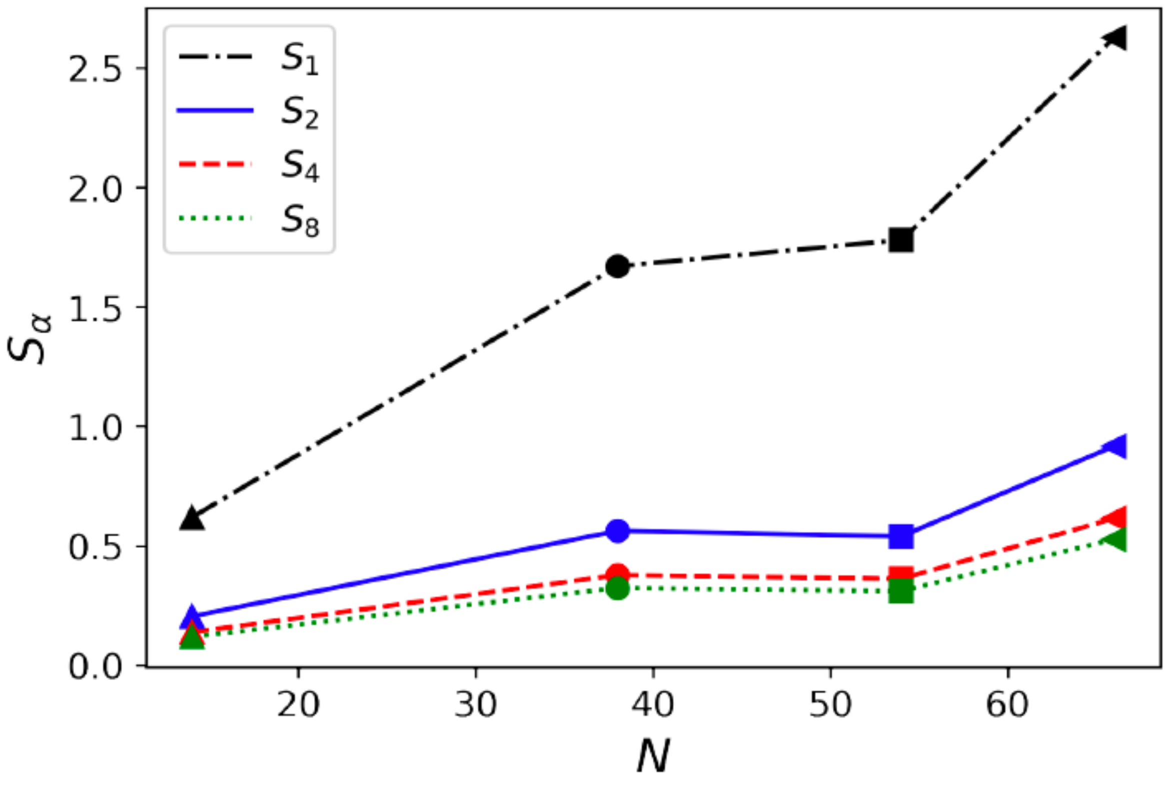
Entanglement entropies proportional to particle number fluctuation

[Chenyi Gu, TP et al, in prep]

Entanglement entropies for neutron matter

(Interaction: Minnesota potential)





Entanglement entropies proportional to particle number fluctuation; with N = 14 (triangle up), N = 38 (circle), N = 54 (square), N = 66 (triangle left)

Entanglement entropies follow volume laws; possibly some shell effects visible

[Chenyi Gu, TP et al, in prep]

Intermission

- Obtained analytical expressions for entanglement entropy and number variation for weakly interacting systems via coupled-cluster doubles
- $S_\alpha \propto (\Delta N)^2$ expected to hold generally for nuclei
- General arguments for nuclei: volume law for entanglement entropy
- Results confirmed by pairing model and neutron matter

How can one reduce entanglement?

Renormalization of correlations in coupled-cluster theory

Coupled cluster theory: Expansion in particle-hole correlations; CCSD economical; captures about 90% of the correlation energy; $\mathrm{e}^{T}|\psi\rangle = e^{T_1+T_2+T_3+\cdots}|\psi\rangle$

Proposal: Apply Lepage's insights for renormalization to many-body computations

- CCSD includes 1p-1h, 2p-2h but lacks 3p-3h correlations
- Hypothesis: Energy gain from 3p-3h are dominated by short-range correlations; renormalize via three-body contact, following Lepage (1997)
- See Bedaque, Hammer, van Kolck, Nucl. Phys. A 64

Interaction	Name	c_E
A	1.8/2.0(EM)	−0.12 [52]
A renorm.		−0.0665
B	ΔNNLO$_{\rm GO}$(394)	−0.002 [67]
B renorm.		0.11

	Interaction and method				Exp.
	A renorm. CCSD	A Λ-CCSD(T)	B renorm. CCSD	B CCSDT-1	
^{16}O	127.8	127.8	127.5	127.5	127.62
^{24}O	166	165	169	169	168.96
^{40}Ca	346	347	341	346	342.05
^{48}Ca	420	419	419	420	416.00
^{78}Ni	642	638	636	639	641.55
^{90}Zr	798	795	777	782	783.90
^{100}Sn	842	836	816	818	825.30

Zhonghao Sun, Charles Bell, G. Hagen, TP, arXiv:2205.12990

Why does it work?

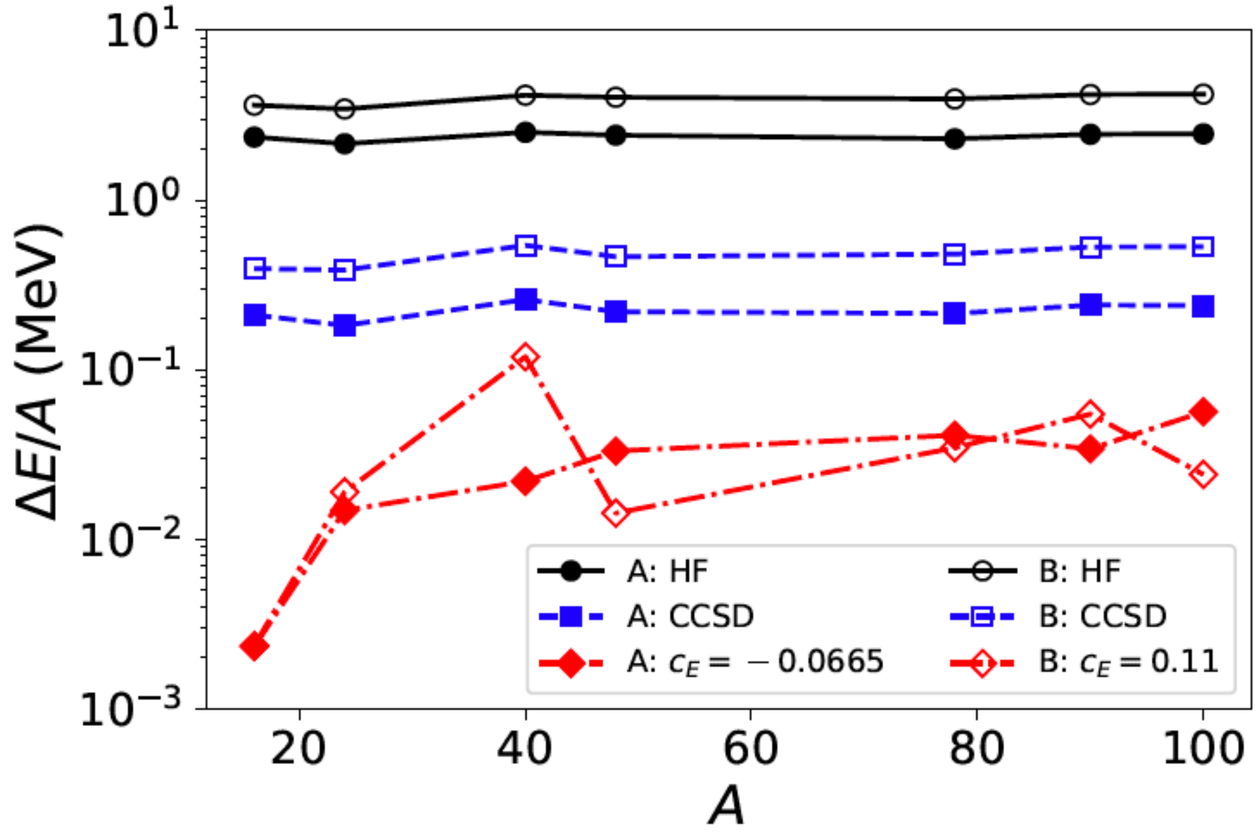
Three-body scattering equation
[Bedaque, Hammer, van Kolck, Nucl. Phys. A 646, 444 (1999); Phys. Rev. Lett. 82, 463 (1999).]

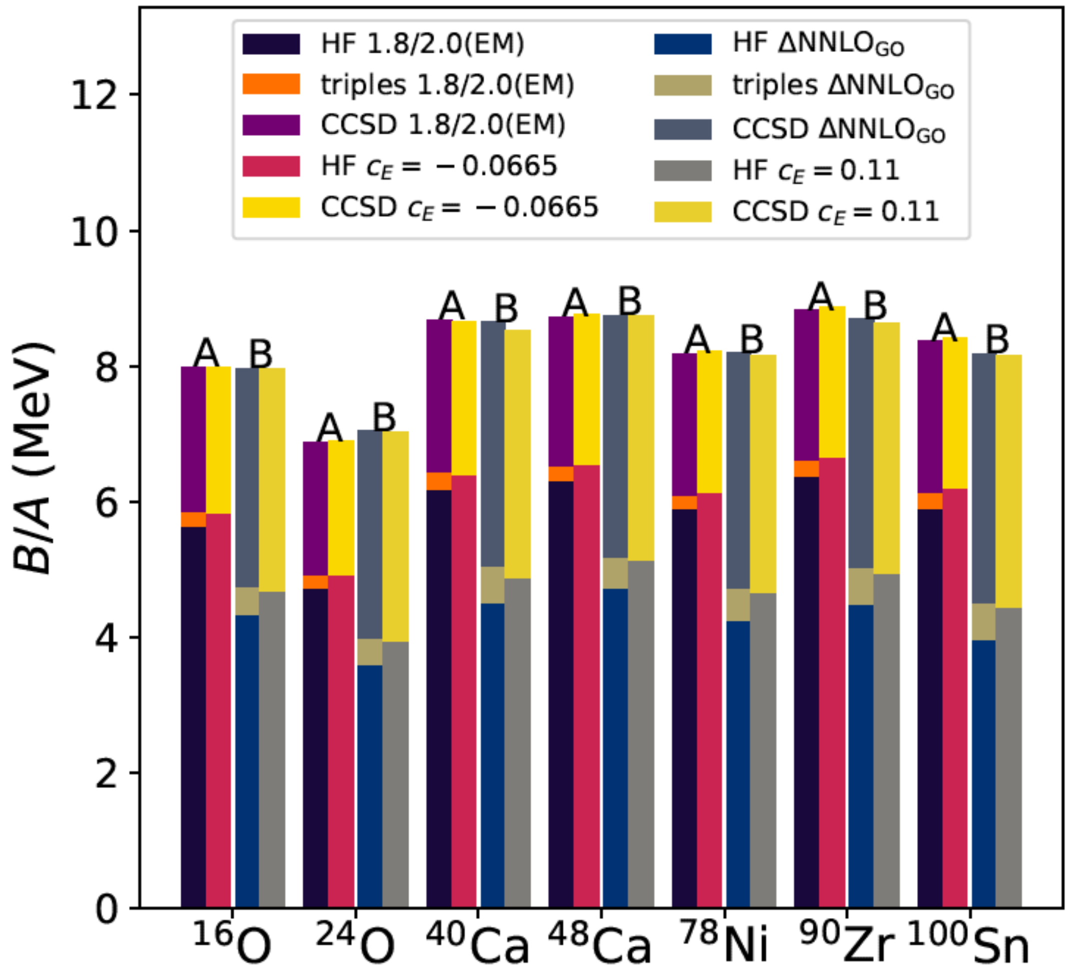
$$t(k,p) = \frac{mg^2}{pk} \ln\left(\frac{p^2+pk+k^2-mE}{p^2-pk+k^2-mE}\right) + h + \frac{2\lambda}{\pi}\int_0^\Lambda dq \frac{t(k,q)q^2}{-\frac{1}{a_2}+\sqrt{\frac{3q^2}{4}-mE}} \left[\frac{1}{pq}\ln\left(\frac{p^2+pq+q^2-mE}{p^2-pq+q^2-mE}\right) + \frac{h}{mg^2}\right]$$

- Two-body physics RG invariant (scattering length a_2 enters)
- Variation of three-body cutoff Λ requires three-body contact (denoted as h)

Thought experiment: Removing triples excitations corresponds to reducing three-body cutoff Λ to Fermi momentum.

How does it work?



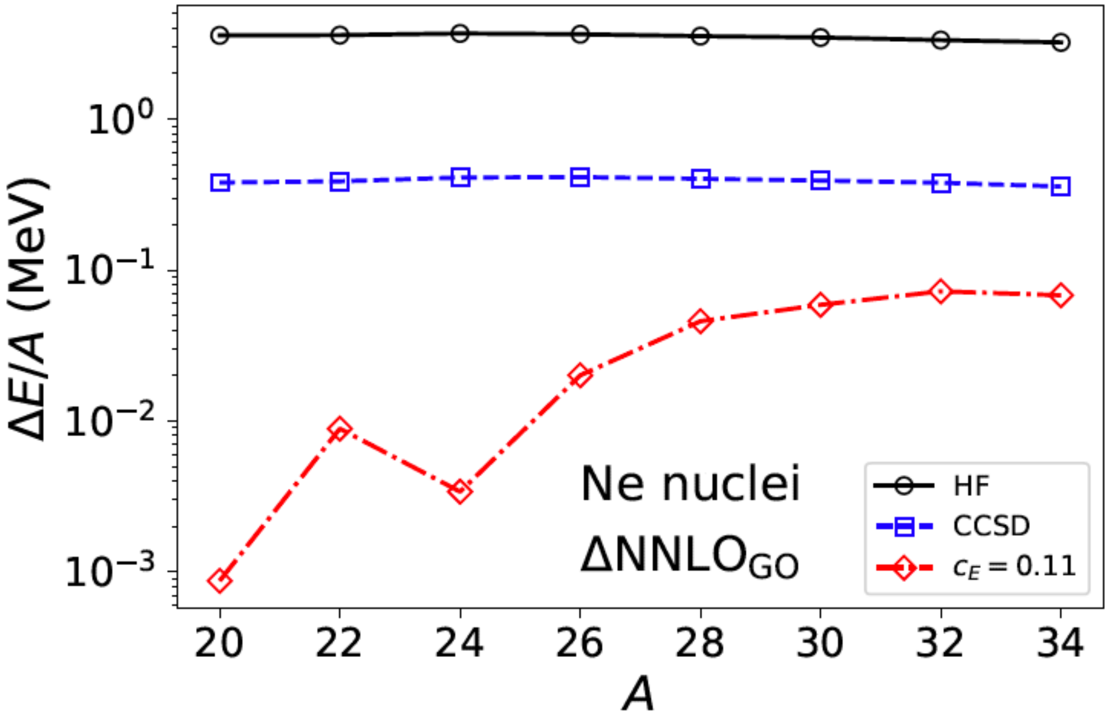


- ΔE = differences to full triples
- Systematic ("order-of-magnitude") improvement from renormalization

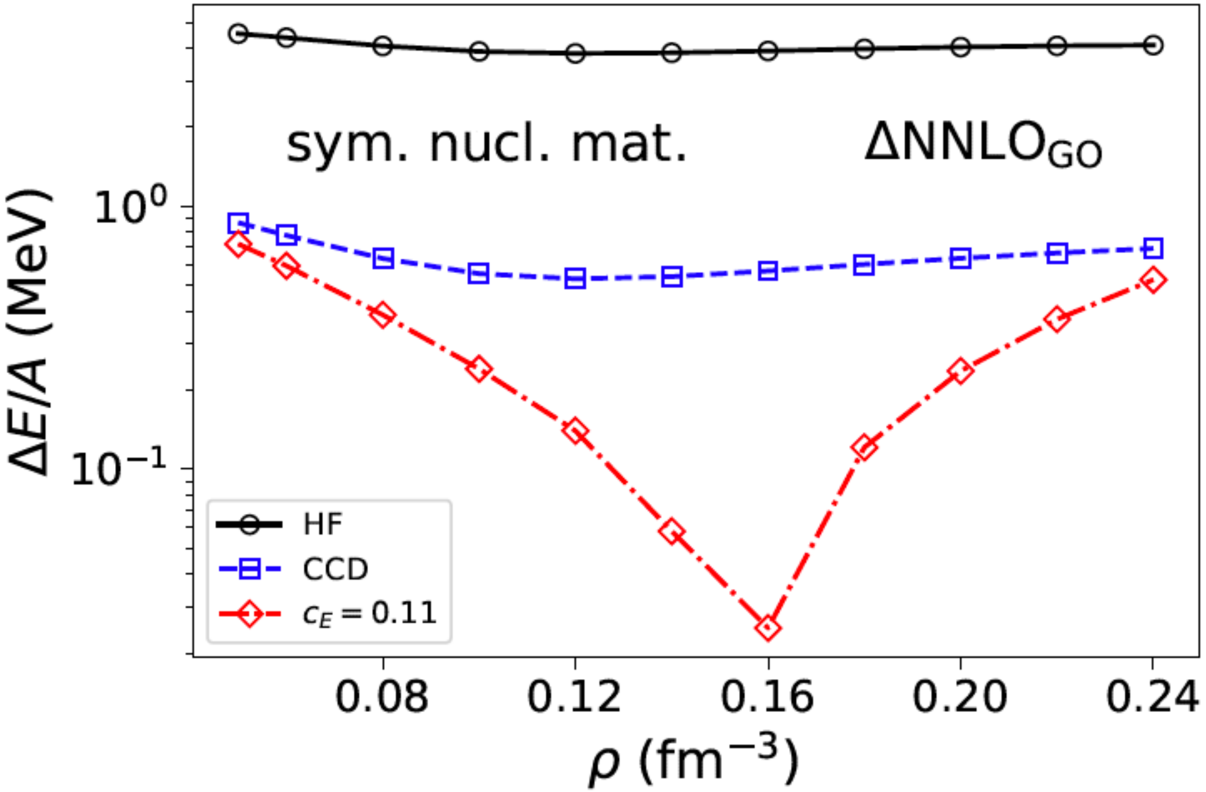
Energy from renormalization essentially goes to HF

Zhonghao Sun, Charles Bell, G. Hagen, TP, arXiv:2205.12990

Weakly bound nuclei and nuclear matter



Renormalization less accurate as the dripline is approached: dilute neutron densities



Nuclear matter only accurate around saturation as $\Delta E \propto c_E\, \rho^3$ in HF

Proposed to link correlations to the renormalization group: Renormalization reduces entanglement

Zhonghao Sun, Charles Bell, G. Hagen, TP, arXiv:2205.12990

Summary

- Studied entanglement in nuclear systems
- Analytical expressions for entanglement entropies between hole and particle space
- Volume laws for pairing model and nuclear matter
- How to reduce entanglement?
- Renormalize Hamiltonian when 3p-3h excitations are removed
- Proposal links particle-hole excitations to ideas from EFT and RG