

# METHODS FOR SYSTEMATIC STUDY OF NUCLEAR STRUCTURE IN HIGH-ENERGY COLLISIONS

OR: CHANGING NUCLEI BY SHIFTING NUCLEONS

Matthew Luzum

Reference: ML, Mauricio Hippert, Jean-Yves Ollitrault; Eur.Phys.J.A 59 (2023) 5, 110; arXiv:2302.14026

Code available at <https://gitlab.com/mhippert/isobar-sampler>

University of São Paulo

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# MOTIVATION

- Most initial of stages: nuclei before collision
- $\Rightarrow$  Nuclear structure affects all subsequent stages
- Ultrarelativistic collisions probe nuclei in a complementary way to low-energy experiments
- $\Rightarrow$  systematic study of nuclear structure in high-energy collisions is of significant interest to multiple communities

# INTRODUCTION

- Systematic study of nuclear properties requires changing nuclear parameters and studying how observables change
- Small changes in parameters  $\implies$  small change in observables
- $\implies$  Huge statistics required?
- No! It's possible to determine **change** in observables (or relative observable ratios) much more precisely than absolute value

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## PROCEDURE USED UNTIL NOW

- 1 Choose parameter values
- 2 Sample distribution to generate nuclear configurations
- 3 Collide nuclei and compute observables
- 4 Choose new set of nuclear parameters
- 5 Generate new set of nuclear configurations
- 6 Perform collisions and compute observables
- 7 Determine change in observables

## BETTER PROCEDURE

- 1 Generate discrete nuclear configurations **once**.
- 2 For each desired parameter set, modify configurations to obey new distribution by making small **shifts to nucleon positions**
  - Statistical uncertainty in observable ratios can be drastically reduced
  - Can study short-range **correlations** in addition to 1-body distribution

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- 1 PREPARATION OF SPHERICAL NUCLEUS
- 2 MODIFYING 1-BODY DISTRIBUTION
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## ASIDE: STEP + GAUSS DISTRIBUTION

- In our code, we use an alternative to a Woods-Saxon
- Not necessary, but has nice properties and makes some things easier

- Nucleon position is sum of two random vectors sampled from:

① 3D step  $P_s(\mathbf{x}) \sim \Theta(R_s - r)$

② 3D Gaussian  $P_g(\mathbf{x}) \sim e^{-\frac{r^2}{2w^2}}$

- Rough rule of thumb:

$$R_s(R, a) \simeq R \left[ 1 + 1.5 \left( \frac{a}{R} \right)^{1.8} \right]$$

$$w(R, a) \simeq 1.83 a$$

$$\rho_c(\mathbf{x}) = \int P_s(\mathbf{z}) P_g(\mathbf{x} - \mathbf{z}) d^3z$$

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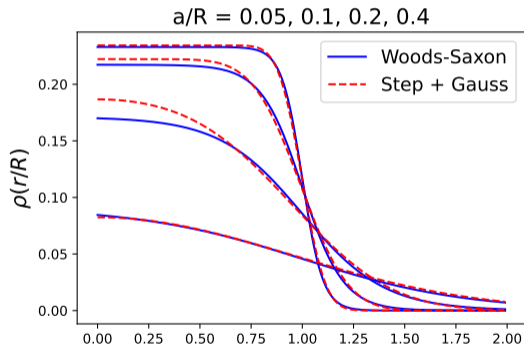
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# STEP+GAUSS DISTRIBUTION ADVANTAGES

## BENEFITS OF STEP+GAUSS

- Can directly modify Woods-Saxon parameters  $R$ ,  $a$  without using the following numerical methods
- Fast/easy to sample
- Nice analytic properties — smooth at origin
- Trivial relation between point nucleon density and charge density

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# CHANGING NUCLEAR SHAPE

- 1-body nucleon distribution parameterized as

$$\rho(r) \propto \frac{1}{1 + e^{\frac{r-R}{a}}}$$
$$\tilde{\rho}(r, \theta, \phi) \propto \frac{1}{1 + e^{\frac{r-R-R \sum_{\ell,m} \beta_{\ell,m} Y_{\ell,m}}{a}}} = \rho(r - R \sum_{\ell,m} \beta_{\ell,m} Y_{\ell,m})$$

- Define continuous parameter  $t$  that takes you from spherical ( $t = 0$ ) to desired deformed distribution ( $t = 1$ )

$$\tilde{\rho}(\vec{x}, t) \equiv \rho(r - t \sum_{\ell,m} R \beta_{\ell,m} Y_{\ell,m})$$

- Idea: change nuclear properties by shifting the position of nucleons

$$\implies \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$$

- Start with uncorrelated nucleons satisfying  $\rho(r)$ , end with uncorrelated nucleons satisfying  $\rho(r - R \sum_{\ell,m} \beta_{\ell,m} Y_{\ell,m})$

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- One solution (at  $t = 0$ ):

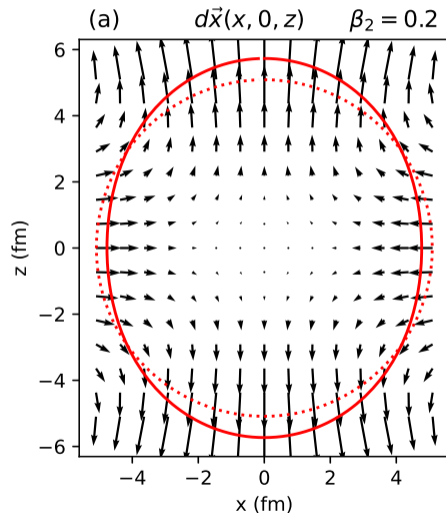
$$\vec{v} = \nabla \Phi(\vec{x})$$

$$\Phi = \sum R \beta_{\ell, m} f_{\ell, m}(r) Y_{\ell, m}$$

$$0 = f''_{\ell, m} + f'_{\ell, m} \left( \frac{2}{r} + \frac{\rho'}{\rho} \right) - \frac{\ell(\ell+1)}{r^2} f_{\ell, m} - \frac{\rho'}{\rho}$$

$$0 = f_{\ell, m}(r \rightarrow 0)$$

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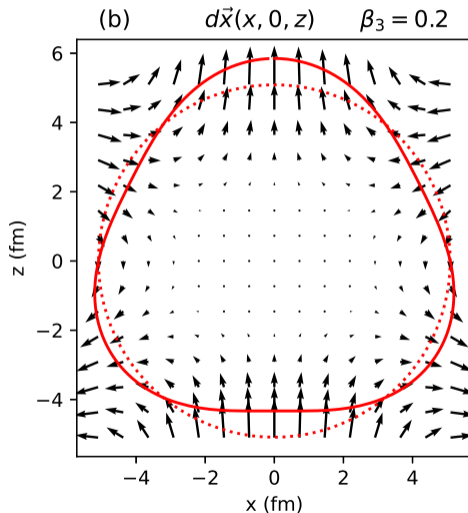
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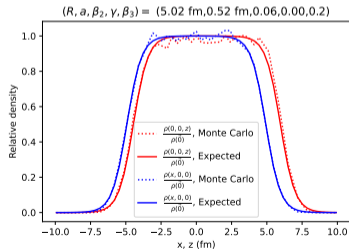
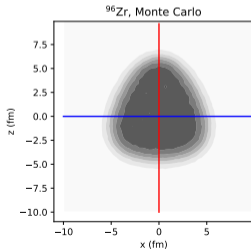
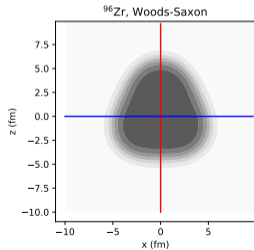
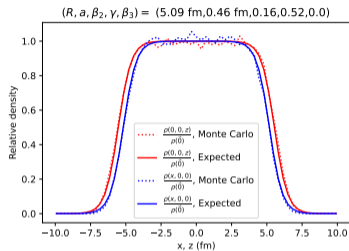
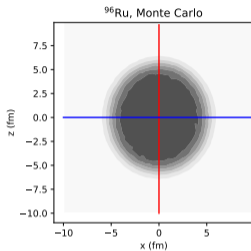
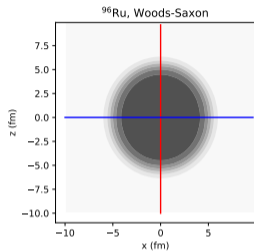
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# NUMERICAL RESULTS (100K NUCLEI)



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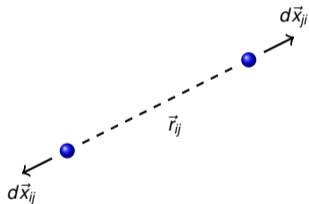
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# SHORT-RANGE CORRELATIONS

- Short-range interactions cause particles to be correlated

$$\rho_2(\vec{x}_1, \vec{x}_2) = \rho(\vec{x}_1)\rho(\vec{x}_2) [1 + C(\vec{r}_{12})]$$

- Idea: induce correlation  $C$  from uncorrelated set by shifting particles



$$d\vec{x}_i = \sum_{j \neq i} d\vec{x}_{ij} = \sum_{j \neq i} \frac{1}{2} (\tilde{r}_{ij} - r_{ij}) \hat{r}_{ij}$$

# FINDING $dr = \tilde{r} - r$

- Conserve pairs:

$$\int_0^r d^3 r' = \int_0^{\tilde{r}} d^3 r' (1 + C(\vec{r}'))$$

- Invert relation to solve for  $\tilde{r}$
- Simple example: step function with variable length  $C_{\text{length}} \geq 0$  and strength  $C_{\text{strength}} \geq -1$

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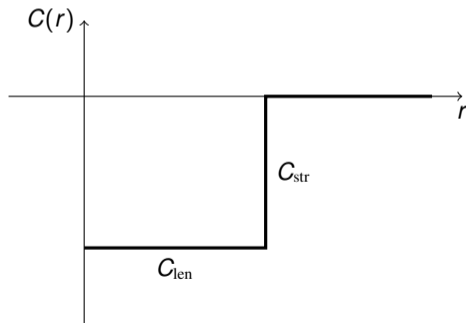
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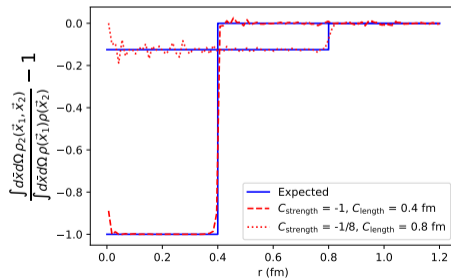
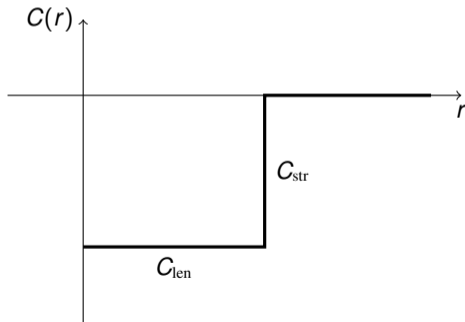


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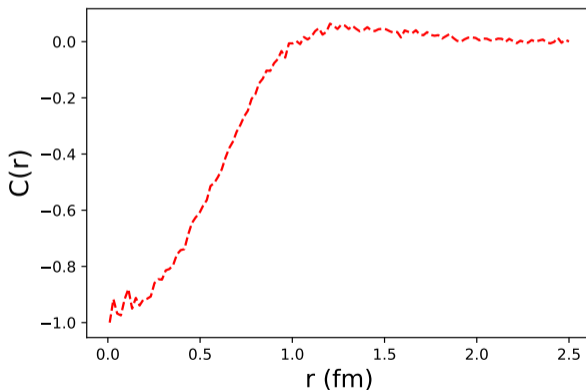
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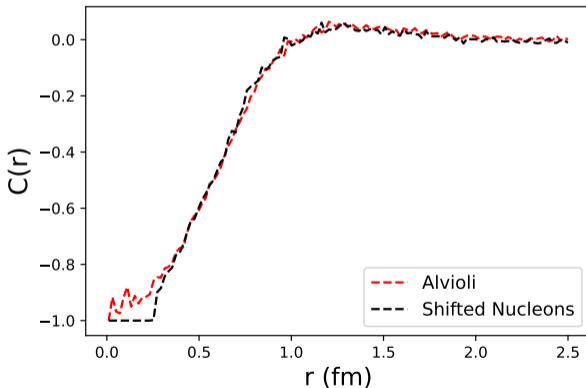
# REALISTIC CORRELATIONS

- Can also implement arbitrary numerical correlation function
- E.g., extracted from 10000  $^{96}\text{Ru}$  configurations generated from realistic 2- and 3-body interactions Hammelmann, Soto-Ontoso, Alvioli, Elfner, Strikman; Phys. Rev. C 101, 061901(R)



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## ADVANTAGES

Compared to usual implementation (i.e., “exclusion radius”):

- Can study correlation of arbitrary shape
- Compatible with any 1-body distribution (no problems with triaxial nuclei)
- Better control over 2-body and 1-body distributions

Compared to sophisticated Monte-Carlo of Alvioli, Strikman, *et al.*:

- Faster and easier
- Anyone can generate their own configurations
- (But lacks 3-body correlations)

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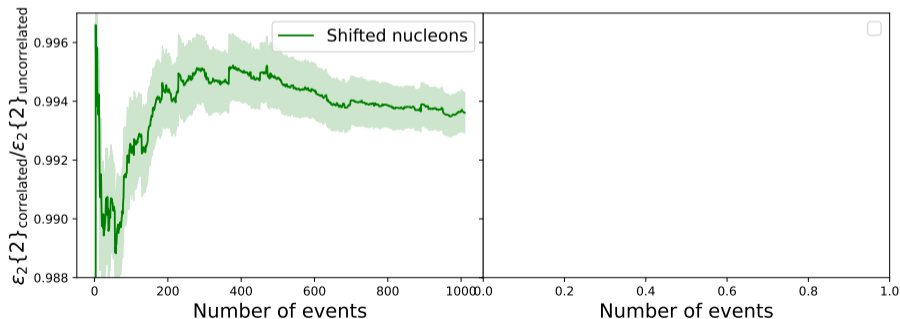
## HOW MUCH BENEFIT CAN YOU GET?

- Simple benchmark test: Trento model at  $b = 0$ .
- Ratio of eccentricities  $\varepsilon_n\{k\}$  with realistic correlation / no correlation
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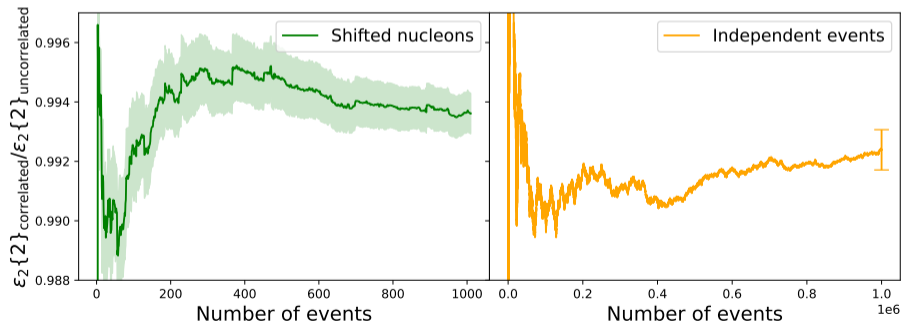
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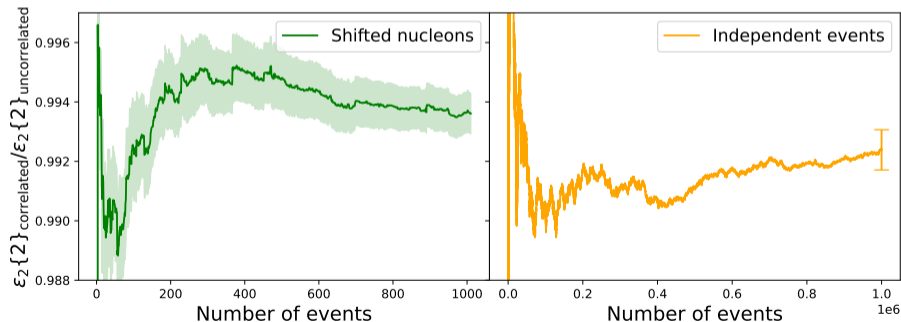
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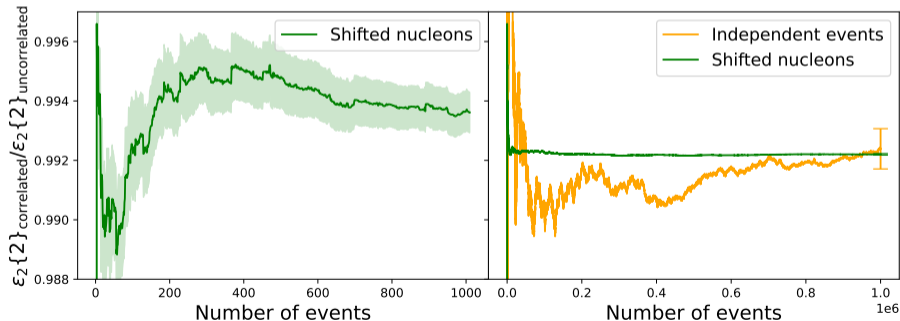
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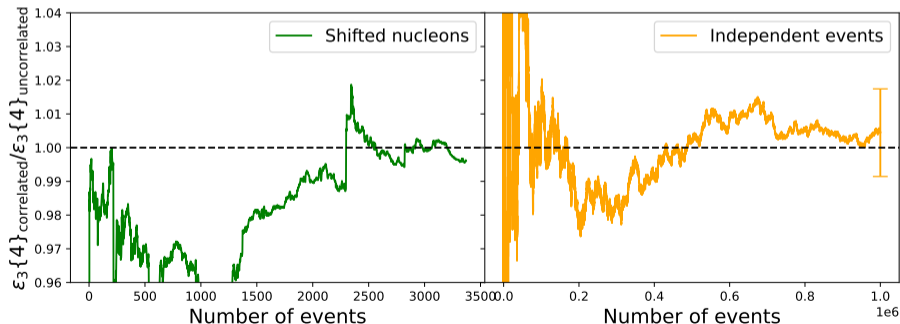
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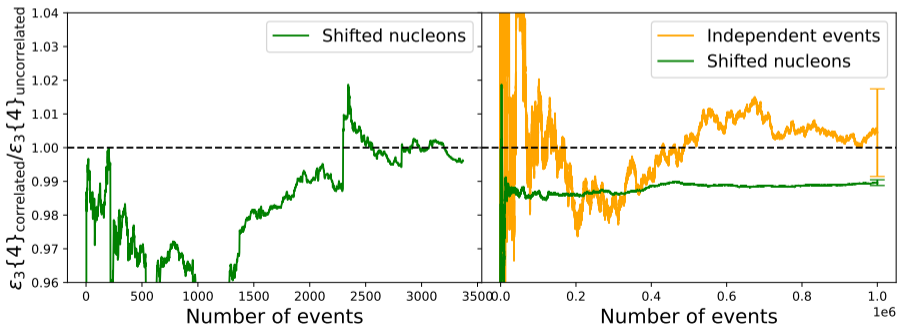
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## OTHER BENCHMARKS (PARTICIPANT GLAUBER MODEL)

Par.	Param. Change	$\varepsilon_2\{2\}$ Change	Improv. Factor	Avg. Shift
$C_{\text{str}} C_{\text{len}}^3$	$(0.2 \text{ fm})^3$	0.13%	2900	0.002 fm
$C_{\text{str}} C_{\text{len}}^3$	$\times 2$	0.27%	1100	0.005 fm
$C_{\text{str}} C_{\text{len}}^3$	$\times 4$	0.53%	350	0.009 fm
$C_{\text{str}} C_{\text{len}}^3$	$(0.4 \text{ fm})^3$	1.1%	180	0.017 fm
$C_{\text{str}} C_{\text{len}}^3$	$\times 2$	2.0%	98	0.032 fm
$C_{\text{str}} C_{\text{len}}^3$	$\times 4$	3.8%	54	0.059 fm
$C_{\text{str}} C_{\text{len}}^3$	$(0.8 \text{ fm})^3$	7.3%	25	0.11 fm
$C_{\text{str}} C_{\text{len}}^3$	$\times 2$	14%	13	0.19 fm

### TAKEAWAYS

- Significant improvement possible
- Main limitation: nucleon shift can change participant  $\leftrightarrow$  spectator
- Smaller differences in nuclei  $\implies$  larger improvement factor
- Exact numbers will depend on model, centrality, etc.

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Par.	Param. Change	$\varepsilon_n\{2\}$ Change	Improv. Factor	Avg. Shift
$\beta_2$	0.005	0.02%	170	0.008 fm
$\beta_2$	0.01	0.10%	100	0.02 fm
$\beta_2$	0.02	0.39%	42	0.03 fm
$\beta_2$	0.05	2.3%	12	0.08 fm
$\beta_2$	0.1	8.8%	4.7	0.17 fm
$\beta_2$	0.2	31%	2.1	0.33 fm
$\beta_3$	0.01	0.05%	79	0.01 fm
$\beta_3$	0.05	1.6%	13	0.06 fm
$\beta_3$	0.1	6.3%	5.0	0.12 fm
$\beta_3$	0.2	23%	2.2	0.25 fm

### TAKEAWAYS

- Smaller efficiency gain for angular deformation (for same average shift distance)
- (Particles near edge of nucleus have larger than average shift)

# SUMMARY

- Can significantly reduce statistical demands by correlating statistical fluctuations — change nuclear properties by shifting nucleons
- Opens many more opportunities for systematic study of nuclear structure
- Can study arbitrary Woods-Saxon parameters ( $R, a, \{\beta_{\ell,m}\}$ ) and short-range correlation function  $C(\vec{r})$
- Statistical improvements depend on context — better advantage for smaller changes in nuclei — but always an improvement over standard method, and potentially dramatic speedup
- Python code to generate nuclei available at <https://gitlab.com/mhippert/isobar-sampler>
- Warning: must synchronize other fluctuations in collision model — impact parameter, orientation of nuclei, etc.

# EXTRA SLIDES

# VALID CORRELATION FUNCTIONS

- Note that the number of pairs is fixed:

$$\rho(\vec{x}_1)\rho(\vec{x}_2) [1 + C(\vec{r}_{12})] = \rho_2(\vec{x}_1, \vec{x}_2) \\ \Rightarrow \int d^3x_1 d^3x_2 \rho(\mathbf{x}_1)\rho(\mathbf{x}_2)C(\vec{r}_{12}) = 0$$

- Respecting sum rule important for maintaining fixed 1-body distribution
- If nominal short-range correlation doesn't satisfy, we add constant

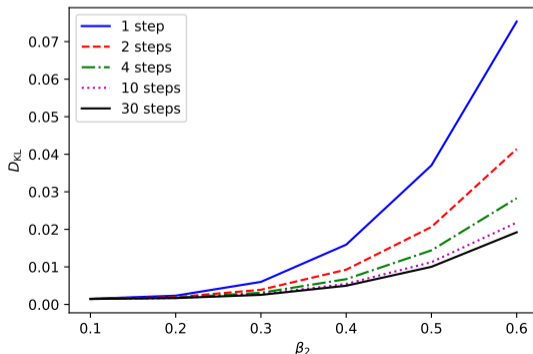
$$C(r) = C_{\text{short}}(r) + C_{\infty} \\ C_{\infty} \simeq -C_{\text{vol}} \int d^3x \rho(\mathbf{x})^2$$

# QUANTIFYING 1-BODY DENSITY

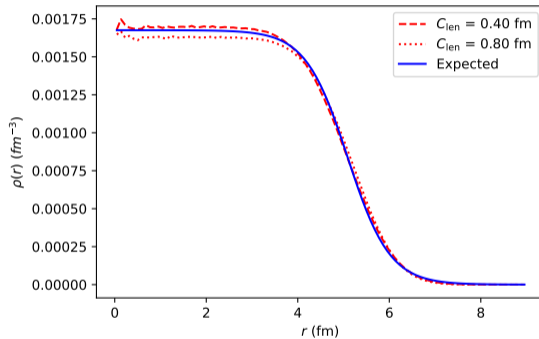
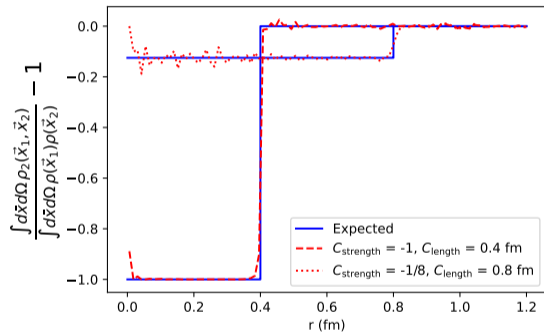
A natural way to compare probability distributions is the Kullback–Leibler (KL) divergence

$$D_{\text{KL}}(\rho_1||\rho_2) \equiv \int d^3x \rho_1(\mathbf{x}) \log \frac{\rho_1(\mathbf{x})}{\rho_2(\mathbf{x})}.$$

Accuracy increases if the nucleon shift is broken into multiple steps.



# 1- AND 2-PARTICLE DENSITIES



# REWEIGHTING METHOD

- Can probe different points in parameter space with *no* extra simulations by reweighting the collision events. However, it converges very poorly unless the parameter values are very close.
- It is more efficient than shifting nucleons for small changes ( $\Delta\beta \lesssim 0.01$ ), but loses efficacy quickly for larger changes, becoming worse than independent sampling for  $\Delta\beta \gtrsim 0.08$  or  $\Delta(C_{\text{str}} C_{\text{len}}^3) \gtrsim (0.3 \text{ fm})^3$  and rapidly degrading beyond that.

