Nuclear wave functions for HIC: ab initio PGCM

Benjamin Bally

CERN - 13/11/2024





• Collaboration between low- and high-energy nuclear physics



- · Collaboration between low- and high-energy nuclear physics
- Nuclear deformation impacts initial conditions and final state observables Giacalone, PRL 127, 242301 (2021); Bally, PRL 128, 082301 (2022); Jia, PRL 131, 022301 (2023); etc.



- · Collaboration between low- and high-energy nuclear physics
- Nuclear deformation impacts initial conditions and final state observables Giacalone, PRL 127, 242301 (2021); Bally, PRL 128, 082301 (2022); Jia, PRL 131, 022301 (2023); etc.
- Use nuclear structure information to better
 - determine the initial conditions of ultra-relativistic ion-ion collisions
 - understand the results of high-energy experiments



- · Collaboration between low- and high-energy nuclear physics
- Nuclear deformation impacts initial conditions and final state observables Giacalone, PRL 127, 242301 (2021); Bally, PRL 128, 082301 (2022); Jia, PRL 131, 022301 (2023); etc.
- Use nuclear structure information to better
 - determine the initial conditions of ultra-relativistic ion-ion collisions
 - understand the results of high-energy experiments
- Use high-energy experiments to gain knowledge about atomic nuclei properties



- · Collaboration between low- and high-energy nuclear physics
- Nuclear deformation impacts initial conditions and final state observables Giacalone, PRL 127, 242301 (2021); Bally, PRL 128, 082301 (2022); Jia, PRL 131, 022301 (2023); etc.
- Use nuclear structure information to better
 - $\diamond~$ determine the initial conditions of ultra-relativistic ion-ion collisions
 - understand the results of high-energy experiments
- Use high-energy experiments to gain knowledge about atomic nuclei properties
- Projected Generator Coordinate Method (PGCM) in this context

Previous works on heavy-ion collisions

- <u>cea</u>
- PGCM calculations with a phenomenological interaction: ¹²⁹Xe, ¹⁹⁷Au, ²⁰⁸Pb



Bally, PRL 128, 082301 (2022)

• Lattice QCD calculations of atomic nuclei not yet possible



- Lattice QCD calculations of atomic nuclei not yet possible
- Nucleons and pions as relevant degrees of freedom to describe atomic nuclei



- Lattice QCD calculations of atomic nuclei not yet possible
- Nucleons and pions as relevant degrees of freedom to describe atomic nuclei

CERN - 13/11/2024

- Construct nuclear Hamiltonian through Effective Field Theory (EFT)
 Hammer, RMP 92, 025004 (2020)
 - $\diamond~$ Consistent with symmetries of QCD
 - ♦ Power counting $\left(\frac{Q}{\Lambda}\right)^n$
 - Different versions: chiral, pionless, deltafull





- Lattice QCD calculations of atomic nuclei not yet possible
- Nucleons and pions as relevant degrees of freedom to describe atomic nuclei



• Solve the many-body Schrödinger equation in a controlled manner to a target accuracy

$$H|\Psi\rangle = E|\Psi\rangle$$

CERN - 13/11/2024







Originally formulated to describe fission

Hill and Wheeler, Phys. Rev. 89, 1102 (1953)



- Originally formulated to describe fission Hill and Wheeler, Phys. Rev. 89, 1102 (1953)
- Nowadays, used for many applications
 - Low-energy spectroscopy (excitation energies, electromagnetic transitions)
 - Nuclear matrix elements for the neutrinoless double-beta decay Belley, PRL 132, 182502 (2024)
 - Initial conditions of ultra-relativistic light-ion collisions

Giacalone, arXiv:2402.05995 (2024); Giacalone, arXiv:2405.20210 (2024)



- Originally formulated to describe fission
 Hill and Wheeler, Phys. Rev. 89, 1102 (1953)
- Nowadays, used for many applications
 - Low-energy spectroscopy (excitation energies, electromagnetic transitions)
 - Nuclear matrix elements for the neutrinoless double-beta decay Belley, PRL 132, 182502 (2024)
 - Initial conditions of ultra-relativistic light-ion collisions Giacalone, arXiv:2402.05995 (2024); Giacalone, arXiv:2405.20210 (2024)
- Traditionally, employed with phenomenological nuclear interactions
- Recently, use of chiral interaction obtained from EFT



• Minimization of the energy

$$\delta\left(\langle \Phi | H | \Phi \rangle\right) = 0$$

• $|\Phi\rangle \equiv$ product state (Slater determinant or Bogoliubov quasi-particle state)

cea

• Minimization of the energy

$$\delta\left(\langle \Phi | H | \Phi \rangle\right) = 0$$

- $|\Phi\rangle \equiv$ product state (Slater determinant or Bogoliubov quasi-particle state)
- Use of symmetry-breaking state

$$\left|\Phi\right\rangle = \sum_{ZNJM\pi}\sum_{\epsilon}c_{\epsilon}^{ZNJM\pi}\left|\Psi_{\epsilon}^{ZNJM\pi}\right\rangle$$

• Minimization of the energy

$$\delta\left(\langle \Phi | H | \Phi \rangle\right) = 0$$

- $|\Phi\rangle \equiv$ product state (Slater determinant or Bogoliubov quasi-particle state)
- Use of symmetry-breaking state

$$\left|\Phi\right\rangle = \sum_{ZNJM\pi}\sum_{\epsilon}c_{\epsilon}^{ZNJM\pi}\left|\Psi_{\epsilon}^{ZNJM\pi}\right\rangle$$



Cez

• Minimization of the energy

$$\delta\left(\langle \Phi | H | \Phi \rangle\right) = 0$$

- $|\Phi\rangle \equiv$ product state (Slater determinant or Bogoliubov quasi-particle state)
- Use of symmetry-breaking state

$$\left|\Phi\right\rangle = \sum_{ZNJM\pi}\sum_{\epsilon}c_{\epsilon}^{ZNJM\pi}\left|\Psi_{\epsilon}^{ZNJM\pi}\right\rangle$$







• Explore the energy surface performing constrained minimization

 $\delta(\langle \Phi(q)|H-\lambda Q|\Phi(q)\rangle) = 0 \quad \text{with} \quad \langle \Phi(q)|Q|\Phi(q)\rangle = q$



• Explore the energy surface performing constrained minimization

 $\delta(\langle \Phi(q) | H - \lambda Q | \Phi(q) \rangle) = 0 \quad \text{with} \quad \langle \Phi(q) | Q | \Phi(q) \rangle = q$





• Explore the energy surface performing constrained minimization

 $\delta(\langle \Phi(q)|H - \lambda Q | \Phi(q) \rangle) = 0 \quad \text{with} \quad \langle \Phi(q)|Q | \Phi(q) \rangle = q$





• Explore the energy surface performing constrained minimization

 $\delta\left(\langle \Phi(q) | H - \lambda Q | \Phi(q) \rangle\right) = 0 \quad \text{with} \quad \langle \Phi(q) | Q | \Phi(q) \rangle = q$







Linear superposition of symmetry-projected states



• We consider the more general wave functions

$$|\Psi_{\epsilon}^{\sigma M}\rangle = \sum_{qK} f_{\epsilon,qK}^{\sigma M} P_{MK}^{\sigma} |\Phi(q)\rangle \quad \text{where} \quad \sigma \equiv Z, N, J, \pi$$



Linear superposition of symmetry-projected states

<u>cea</u>

• We consider the more general wave functions

$$|\Psi_{\epsilon}^{\sigma M}\rangle = \sum_{qK} f_{\epsilon,qK}^{\sigma M} P_{MK}^{\sigma} |\Phi(q)\rangle \quad \text{where} \ \sigma \equiv Z, N, J, \pi$$

• Weights $f_{\epsilon,qK}^{\sigma M}$ determined by a variational principle

$$\frac{\delta}{\delta f_{\epsilon,qK}^{\sigma M \star}} \left(\langle \Psi_{\epsilon}^{\sigma M} | H | \Psi_{\epsilon}^{\sigma M} \rangle \right) = 0$$



Linear superposition of symmetry-projected states

<u>cea</u>

• We consider the more general wave functions

$$|\Psi_{\epsilon}^{\sigma M}\rangle = \sum_{qK} f_{\epsilon,qK}^{\sigma M} P_{MK}^{\sigma} |\Phi(q)\rangle \quad \text{where} \quad \sigma \equiv Z, N, J, \pi$$

• Weights $f_{\epsilon,qK}^{\sigma M}$ determined by a variational principle

$$\frac{\delta}{\delta f_{\epsilon,qK}^{\sigma M \star}} \left(\langle \Psi_{\epsilon}^{\sigma M} | H | \Psi_{\epsilon}^{\sigma M} \rangle \right) = 0$$





- The method is exact for the deuteron Bally, arXiv.2410.03356 (2024)
- Relative error of 1-2% for ³H and ^{3,4}He (preliminary) Bally, in preparation (2025)

Recent developments



- The method is exact for the deuteron Bally, arXiv.2410.03356 (2024)
- Relative error of 1-2% for ³H and ^{3,4}He (preliminary) Bally, in preparation (2025)
- New methods:
 - \diamond PGCM + Perturbation Theory (PT)

Frosini, EPJA 58, 62-63-64 (2022)

◊ PGCM + In-Medium Similarity Renormalization Group (IMSRG) Zhou, arXiv:2410.23113 (2024)

Sampling of nucleons

• Here: deformed one-body density at the average deformation \bar{q} of the PGCM ground state

$$\rho_{\bar{q}}^{(1)}(r_1) = \frac{\langle \Phi(\bar{q}) | a_{r_1}^+ a_{r_1} P^Z P^N | \Phi(\bar{q}) \rangle}{\langle \Phi(\bar{q}) | P^Z P^N | \Phi(\bar{q}) \rangle}$$



Sampling of nucleons

• Here: deformed one-body density at the average deformation \bar{q} of the PGCM ground state

$$\rho_{\bar{q}}^{(1)}(r_1) = \frac{\langle \Phi(\bar{q}) | a_{r_1}^+ a_{r_1} P^Z P^N | \Phi(\bar{q}) \rangle}{\langle \Phi(\bar{q}) | P^Z P^N | \Phi(\bar{q}) \rangle}$$

• Near future: one-body and two-body correlated densities

$$\begin{split} \rho^{(1)}(r_1) &= \frac{\langle \Psi_{\epsilon}^{\sigma M} | a_{r_1}^+ a_{r_1} | \Psi_{\epsilon}^{\sigma M} \rangle}{\langle \Psi_{\epsilon}^{\sigma M} | \Psi_{\epsilon}^{\sigma M} \rangle} \\ \rho^{(2)}(r_1, r_2) &= \frac{\langle \Psi_{\epsilon}^{\sigma M} | a_{r_1}^+ a_{r_2}^+ a_{r_2} a_{r_1} | \Psi_{\epsilon}^{\sigma M} \rangle}{\langle \Psi_{\epsilon}^{\sigma M} | \Psi_{\epsilon}^{\sigma M} \rangle} \end{split}$$

 \rightarrow all ingredients already computed, just need to combine them together

Sampling of nucleons

• Here: deformed one-body density at the average deformation \bar{q} of the PGCM ground state

$$\rho_{\bar{q}}^{(1)}(r_1) = \frac{\langle \Phi(\bar{q}) | a_{r_1}^+ a_{r_1} P^Z P^N | \Phi(\bar{q}) \rangle}{\langle \Phi(\bar{q}) | P^Z P^N | \Phi(\bar{q}) \rangle}$$

• Near future: one-body and two-body correlated densities

$$\begin{split} \rho^{(1)}(r_1) &= \frac{\left\langle \Psi^{\sigma M}_{\epsilon} | a^+_{r_1} a_{r_1} | \Psi^{\sigma M}_{\epsilon} \right\rangle}{\left\langle \Psi^{\sigma M}_{\epsilon} | \Psi^{\sigma M}_{\epsilon} \right\rangle} \\ \rho^{(2)}(r_1, r_2) &= \frac{\left\langle \Psi^{\sigma M}_{\epsilon} | a^+_{r_1} a^+_{r_2} a_{r_2} a_{r_1} | \Psi^{\sigma M}_{\epsilon} \right\rangle}{\left\langle \Psi^{\sigma M}_{\epsilon} | \Psi^{\sigma M}_{\epsilon} \right\rangle} \end{split}$$

 \rightarrow all ingredients already computed, just need to combine them together

• Ultimate goal: A-body correlated density (as in NLEFT)

$$\rho^{(A)}(r_1,\ldots,r_A) = \frac{\langle \Psi_{\epsilon}^{\sigma M} | a_{r_1}^+ \ldots a_{r_A}^+ a_{r_A} \ldots a_{r_1} | \Psi_{\epsilon}^{\sigma M} \rangle}{\langle \Psi_{\epsilon}^{\sigma M} | \Psi_{\epsilon}^{\sigma M} \rangle}$$





 $\operatorname{CERN-TH-2024-021}$

The unexpected uses of a bowling pin: exploiting ²⁰Ne isotopes for precision characterizations of collectivity in small systems

Giuliano Giacalone,^{1, *} Benjamin Bally,² Govert Nijs,³ Shihang Shen,⁴

Thomas Duguet,^{5,6} Jean-Paul Ebran,^{7,8} Serdar Elhatisari,^{9,10} Mikael Frosini,¹¹ Timo A. Lähde,^{12,13}

Dean Lee,¹⁴ Bing-Nan Lu,¹⁵ Yuan-Zhuo Ma,¹⁴ Ulf-G. Meißner ^{10,16,17} Jacquelyn Noronha-Hostler,¹⁸ Christopher Plumberg.¹⁹ Tomás R. Rodríguez.²⁰ Robert Roth.^{21,22} Wilke van der Schee,^{3,23,24} and Vittorio Somå⁵

CERN-TH-2024-074

Anisotropic flow in fixed-target ²⁰⁸Pb+²⁰Ne collisions as a probe of quark-gluon plasma

 Giuliano Giacalone,^{1,*} Wenbin Zhao,^{2,3,†} Benjamin Bally,⁴ Shihang Shen,⁵

 Thomas Duguet,^{6,7} Jean-Paul Ebran,^{8,9} Serdar Elhatisari,¹⁰ Mikael Frosini,¹¹

 Timo A. Lähde,^{12,13} Dean Lee,¹⁴ Bing-Nan Lu,¹⁵ Yuan-Zhuo Ma,¹⁴ Ulf-G. Meißner,^{16,17,5}

 Govert Nijs,¹⁸ Jacquelyn Noronha-Hostler,¹⁹ Christopher Plumberg,²⁰ Tomás R. Rodríguez,²¹

 Robert Roth,^{22,23} Wilke van der Schee,^{18,24,25} Björn Schenke,^{20,1} Chun Shen,^{27,28,§} and Vittorio Somå⁶

- · Collaboration between low- and high-energy nuclear physics communities
 - ◊ Heavy-ion collisions
 - ♦ Nuclear structure (PGCM)
 - Nuclear structure (NLEFT)



• Chiral Hamiltonian: Hüther N3LO

Hüther et al., PLB 808, 135651 (2019)

• Collective coordinates $q: \beta_{20}, \beta_{22}, \beta_{30}, \beta_{32}$

Chiral Hamiltonian: Hüther N3LO

Hüther et al., PLB 808, 135651 (2019)

• Collective coordinates $q: \beta_{20}, \beta_{22}, \beta_{30}, \beta_{32}$

• Numerical suite TAURUS

Bally, EPJA 57, 69 (2021); Bally, EPJA 60, 62 (2024) Repository: https://github.com/project-taurus





Chiral Hamiltonian: Hüther N3LO

Hüther et al., PLB 808, 135651 (2019)

• Collective coordinates $q: \beta_{20}, \beta_{22}, \beta_{30}, \beta_{32}$

• Numerical suite TAURUS

Bally, EPJA 57, 69 (2021); Bally, EPJA 60, 62 (2024) Repository: https://github.com/project-taurus

• Topaze supercomputer (CEA/CCRT)











- · Relative agreement with experimental data
- Density ~ tetrahedron of four $\alpha\text{-like clusters}$

²⁰Ne: spectroscopy and deformed one-body density





- Good agreement with experimental data
- Spectroscopic moment $Q_s = \langle er^2 Y_{20} \rangle$
- Density ~ 16 O + α

Other example: ²⁴Mg



Bally, EPJA 60, 62 (2024)

- Ground state exhibits large intrinsic triaxial deformation
- Excellent description using χEFT Hamiltonian

- PGCM: efficient method to capture collective correlations in atomic nuclei
- Can be used to better model the initial conditions of high-energy experiments



- PGCM: efficient method to capture collective correlations in atomic nuclei
- Can be used to better model the initial conditions of high-energy experiments
- Predictions for ${}^{16}\text{O} + {}^{16}\text{O}$ and ${}^{16}\text{O} + {}^{208}\text{Pb}$ runs at LHC in 2025



- PGCM: efficient method to capture collective correlations in atomic nuclei
- Can be used to better model the initial conditions of high-energy experiments
- Predictions for ${}^{16}\text{O} + {}^{16}\text{O}$ and ${}^{16}\text{O} + {}^{208}\text{Pb}$ runs at LHC in 2025
- Predictions for possible 20 Ne + 20 Ne and 20 Ne + 208 Pb runs at LHC

- PGCM: efficient method to capture collective correlations in atomic nuclei
- Can be used to better model the initial conditions of high-energy experiments
- Predictions for ${}^{16}\text{O} + {}^{16}\text{O}$ and ${}^{16}\text{O} + {}^{208}\text{Pb}$ runs at LHC in 2025
- Predictions for possible 20 Ne + 20 Ne and 20 Ne + 208 Pb runs at LHC
- In the future: sampling based on the correlated densities
 - $\diamond~$ one-body + two-body densities
 - ◊ A-body density