

Evidence of Hexadecapole Deformation in Uranium-238 at the Relativistic Heavy Ion Collider

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State-of-the-art hydrodynamic simulations of the quark-gluon plasma are unable to reproduce the elliptic flow of particles observed at the BNL Relativistic Heavy Ion Collider (RHIC) in relativistic $^{238}\text{U} + ^{238}\text{U}$ collisions when they rely on information obtained from low-energy experiments for the implementation of deformation in the colliding ^{238}U ions. We show that this is due to an inappropriate treatment of well-deformed nuclei in the modeling of the initial conditions of the quark-gluon plasma. Past studies have identified the deformation of the nuclear surface with that of the nuclear volume, though these are different concepts. In particular, a volume quadrupole moment can be generated by both a surface hexadecapole and a surface quadrupole moment. This feature was so far neglected in the modeling of heavy-ion collisions, and is particularly relevant for nuclei like ^{238}U , which is both quadrupole deformed and hexadecapole deformed. With rigorous input from Skyrme density functional calculations, we show that correcting for such effects in the implementation of nuclear deformations in hydrodynamic simulations restores agreement with BNL RHIC data. This brings consistency to the results of nuclear experiments across energy scales, and demonstrates the impact of the hexadecapole deformation of ^{238}U on high-energy collisions.

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Introduction.—The possibility of exploiting the intrinsic deformed shape of atomic nuclei as a means to broaden the scope of ultrarelativistic nuclear collision programs has materialized with the release of data on the collective flow of hadrons in collisions of ^{238}U nuclei (U + U collisions) at the BNL RHIC [1]. The quadrupole (ellipsoidal) deformation of this nucleus introduces an elliptical anisotropy in the quark-gluon plasma (QGP) formed in head-on (central) U + U collisions, which enhances the elliptical modulation (or elliptic flow, v_2 [2,3]) of the emitted particles in momentum space compared to collisions of less deformed ions, such as ^{197}Au . Effects of this type have been later on identified as well in collisions of other deformed species, namely ^{129}Xe , ^{96}Ru , and ^{96}Zr [4–9]. These observations are of fundamental interest, as they allow us to ask whether signatures of the emergent collective properties of nuclei can be understood consistently across experimental techniques and energy scales.

To answer this question in general, one should first ensure that U + U data are captured by hydrodynamic simulations of the QGP: the deformation of ^{238}U is not only the largest among the collided species so far, but it is arguably also the one that is best understood by low-energy models and experiments. However, quantitative high-energy theory-to-data comparisons have recently led to tensions. Estimates of the elliptic flow resulting from the

linear response to an initial QGP eccentricity, $v_2 = \kappa_2 \varepsilon_2$, show that one obtains an overestimate of U + U data for realistic values of κ_2 and ε_2 [10]. Large-scale IP-Glasma + MUSIC + UrQMD calculations show good agreement with v_2 data across energies and collision species, with the exception of central U + U collisions: again the predicted v_2 overshoots the measurements [11,12]. The issue is corroborated by the model-independent analysis of Ref. [13], arguing that the impact of nuclear deformation can be assessed by comparing mean squared v_2 coefficients between collision systems. This ratio can be expressed as

$$r_{\text{Au,U}}\{2\}^2 \equiv \frac{\langle v_2^2 \rangle_{\text{U+U}}}{\langle v_2^2 \rangle_{\text{Au+Au}}} = \frac{1 + a_0(\beta_{2,\text{U}}^{\text{WS}})^2}{a_1 + a_2 a_0(\beta_{2,\text{Au}}^{\text{WS}})^2}, \quad (1)$$

where $\beta_{2,\text{Au}}^{\text{WS}}$ and $\beta_{2,\text{U}}^{\text{WS}}$ are Woods-Saxon (WS) deformation parameters, defined more precisely below, that reflect the quadrupole deformation of both species, while the coefficients $a_{0,1,2}$ represent robust features of the hydrodynamic description of the QGP [13]. Setting the parameter β_2^{WS} to be equal to the quadrupole deformation reported in low-energy literature, one obtains $r_{\text{Au,U}}\{2\}^2 = 1.78 \pm 0.15$, much larger than 1.49 ± 0.05 , the value measured by the STAR Collaboration for head-on (0%–1% central) collisions [1].

However, Ref. [13] along with *all* past theoretical studies of high-energy U + U collisions assumes that $\beta_{2,U}^{\text{WS}}$ in Eq. (1) can be taken from low-energy spectroscopic data, although the deformation extracted from low-energy experiments and the deformation parameter used in the hydrodynamic models are different quantities [14]. Here, we demonstrate that the magnitude of this difference becomes important for well-deformed nuclei with a significant hexadecapole moment, such as ^{238}U [15,16]. We discuss the difference between these two concepts of nuclear deformation, and show that the presence of a hexadecapole moment modifies the appropriate input for hydrodynamic simulations of the QGP. We compute, then, realistic nucleon densities via state-of-the-art nuclear energy density functional (EDF) theory that are consistent with low-energy experimental information, to show that an appropriate deformation parameter is $\beta_{2,U}^{\text{WS}} \approx 0.25$, significantly lower than implemented in previous hydrodynamic studies. Through new state-of-the-art simulations of U + U and Au + Au collisions, we resolve the tension between high-energy observations and low-energy expectations, demonstrating for the first time the impact of the hexadecapole deformation of a nucleus on high-energy data.

A tale of two deformations.—Much of our understanding of the low-energy structure of nuclei hinges on the notion of deformation: the nuclear density in the intrinsic frame can take a variety of shapes. These are typically characterized via dimensionless multipole moments of the nucleon density $\rho(\mathbf{r})$:

$$\beta_{\ell m} = \frac{4\pi}{3R_0^\ell A} \int d^3r \rho(\mathbf{r}) r^\ell Y_{\ell m}(\theta, \phi), \quad \ell \geq 2, \quad (2)$$

where $R_0 = 1.2A^{1/3}$ fm and $Y_{\ell m}(\theta, \phi)$ is a spherical harmonic. We also define the total deformation at order ℓ : $\beta_\ell^2 = \sum_{m=-\ell}^{+\ell} \beta_{\ell m}^2$. While the intrinsic body-frame multipole moments $\beta_{\ell m}$ are not directly observable, the integral in Eq. (2) is the expectation value of a multipole operator whose matrix elements determine the electromagnetic transition rates between nuclear levels [17]. Under strict assumptions [18], the deformation of an even-even nucleus can be inferred from ground state (g.s.) electric transition rates, $B(E\ell)$:

$$\beta_\ell = \frac{4\pi}{(2\ell + 1)ZR_0^\ell} \sqrt{\frac{B(E\ell)}{e^2}}. \quad (3)$$

Quadrupole deformation ($\ell = 2$) is dominant for essentially all nuclei. Octupole ($\ell = 3$) and hexadecapole ($\ell = 4$) deformations play a role in several regions of the nuclear chart [19–21], but measurements of $\ell > 2$ transition rates are scarce.

The nucleus ^{238}U is the archetype of a well-deformed nucleus for which Eq. (3) holds [22]. The recommended value for the $\ell = 2$ transition is $B(E2) = 12.19 \pm 0.62 \text{ e}^2\text{b}^2$ [23], corresponding to $\beta_{2,U} = 0.287 \pm 0.007$. No direct

measurements of $B(E4)$ are available to date, but several more model-dependent analyses report hexadecapole deformations ranging between 0.1 and 0.2 [24,25]. We consider the most direct information available to be that of Refs. [15,16], which report $\beta_4 \sim 0.124 \pm 0.033$ and $\beta_4 \sim 0.144 \pm 0.007$ based on Coulomb excitation (Coulx) and muonic x rays, respectively. As we will see, theoretical calculations faithfully reproduce the quadrupole deformation of ^{238}U , but favor somewhat larger values of β_4 .

The multipole moments of the odd-Z ^{197}Au cannot be determined from $B(E\ell)$ values. Instead, Ref. [13] proposed a conservative estimate, $\beta_{2,\text{Au}} \in [0.1, 0.14]$, based on the predictions of various models and the deformations of neighboring species. Although not often discussed, models typically predict a nonzero hexadecapole deformation [21,26] for ^{197}Au . For instance, a recent state-of-the-art multireference (MR) EDF calculation finds a triaxial g.s. with $\beta_{2,\text{Au}} = 0.13$ and $\beta_{4,\text{Au}} = 0.056$ [27,28].

Now, hydrodynamic simulations of high-energy collisions require nuclear densities to model the colliding ions. Almost without exception, a Woods-Saxon (WS) parametrization is used [29]:

$$\rho^{\text{WS}}(\mathbf{r}) = \frac{\rho_0}{1 + \exp([r - R(\theta, \phi)]/a)}, \quad (4)$$

where ρ_0 fixes the normalization, a is the surface diffuseness, and the angle-dependent radius reads

$$R(\theta, \phi) = R_d \left[1 + \sum_{\ell=2}^{\ell_{\text{max}}} \sum_{m=-\ell}^{\ell} \beta_{\ell m}^{\text{WS}} Y_{\ell m}(\theta, \phi) \right], \quad (5)$$

where R_d is the half-width radius, and $\beta_{\ell m}^{\text{WS}}$ are shape parameters for which we also define a total β_ℓ^{WS} . What has not been fully appreciated so far is that the multipole moments $\beta_{\ell m}$ of a WS density are not equal to the values of the $\beta_{\ell m}^{\text{WS}}$ used to generate them. The former are linked to expectation values of operators and represent the entire nuclear *volume*, while the latter describe the deformation of the nuclear *surface*. Though tedious, it is possible to express the multipole moments of a WS density as a combined power series in the parameters $\beta_{\ell m}^{\text{WS}}$ and a/R_d . As an example, we give here the expression for the quadrupole moment of a density with a sharp profile ($a = 0$) for which only β_{20}^{WS} and β_{40}^{WS} do not vanish:

$$\beta_{20} = \frac{R_d^2}{R_0^2} \left[\beta_{20}^{\text{WS}} + \frac{2}{7} \sqrt{\frac{5}{\pi}} (\beta_{20}^{\text{WS}})^2 + \frac{12}{7\sqrt{\pi}} \beta_{20}^{\text{WS}} \beta_{40}^{\text{WS}} \right], \quad (6)$$

which is valid up to second order in β_{20}^{WS} and to first order in β_{40}^{WS} , and similar to other equations for liquid-drop-type densities available in the literature [30,31]. Equation (6) shows that if β_{20}^{WS} is large, even a small β_{40}^{WS} will enhance

the mismatch between β_{20} and β_{20}^{WS} . To our knowledge, this subtlety has never been considered in the modeling of ^{238}U nuclei in hydrodynamic simulations of the QGP, although, as we will show, it impacts significantly the predicted v_2 in $\text{U} + \text{U}$ collisions. Considering more exotic shapes with, e.g., finite octupole or triaxial deformation, will lead to additional terms in Eq. (6). The construction of WS densities with predetermined multipole moments is, therefore, a nontrivial task.

Skyrme-HFB calculations.—To find WS parameters that better reflect our knowledge of the structure of ^{197}Au and ^{238}U , we perform Hartree-Fock-Bogoliubov (HFB) calculations based on an EDF. We limit ourselves here to an EDF of the widely used Skyrme type [32], but report on the predictions of 21 different parametrizations to gauge the model spread. These parametrizations come in five families: (i) BSkG1/2 [21,33], (ii) SLy4/5/6 [34], (iii) UNEDF0/1/2 [35–37], (iv) SV-min/bas/07/08/10 [38], and (v) SLy5s1-8 [39]. Together, they are fairly representative of the literature.

We solve the self-consistent Skyrme-HFB equations for each nucleus and each parametrization, relying on a three-dimensional numerical representation of the single-particle wave functions in coordinate space [40]. The solution is a many-body Bogoliubov state that minimizes the total energy, whose one-body density we use to calculate all multipole moments $\beta_{\ell m}$ of the nuclear ground state. We impose a few symmetry restrictions on the nuclear shape (see Supplemental Material [41]), which in practice determines that nonvanishing multipole moments have ℓ and m both even. Then we obtain deformation parameters $\beta_{\ell m}^{\text{WS}}$ by fitting Eq. (4) to the three-dimensional HFB density [49]. The results are shown in Fig. 1, displaying the total quadrupole and hexadecapole parameters $\beta_{\ell=2/4}^{\text{WS}}$ as a function of the corresponding total multipole moments for both ^{197}Au and ^{238}U .

We see that the spread in predictions is modest, meaning these 21 Skyrme parametrizations yield a consistent picture of the structure of these nuclei. As expected, the predicted $\beta_{2,\text{U}}$ agrees well with that deduced from the $B(E2)$ value, also shown in the figure as a gray band. The predicted $\beta_{4,\text{U}}$ have a somewhat larger theoretical spread and are in mild tension with the model-dependent experimental information of Refs. [15,16], which also report values of β_{ℓ}^{WS} . Overall, the values of β_{ℓ} correlate linearly with the values of β_{ℓ}^{WS} , though with slopes differing from unity. This leads to our central result: we see that the values of β_{ℓ}^{WS} are consistently lower than the values of β_{ℓ} for ^{238}U , due to the contribution of the volume hexadecapole deformation to the surface quadrupole deformation. Indeed, we recover $\beta_{2}^{\text{WS}} \approx \beta_2 \approx 0.29$ if we constrain the EDF calculations to $\beta_4 = 0$ and values of β_2 that are compatible with low-energy experiment. Our conclusion is that a realistic WS parametrization of the g.s. density of ^{238}U should have

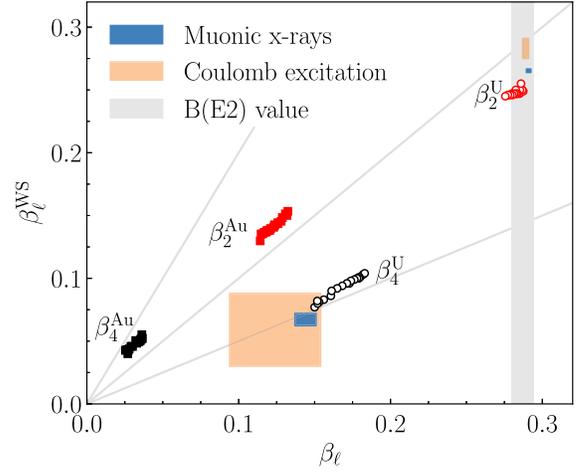


FIG. 1. Total best-fit WS deformation parameters β_{ℓ}^{WS} versus total deformation β_{ℓ} of the mean-field densities obtained with 21 Skyrme parametrizations for ^{197}Au (full squares) and ^{238}U (empty circles), for $\ell = 2$ (red symbols) and $\ell = 4$ (black symbols). The faint gray lines indicate $\beta_{\ell}^{\text{WS}} = \alpha\beta_{\ell}$ for $\alpha = 0.5, 1, \text{ and } 2$.

$\beta_{2,\text{U}}^{\text{WS}} \approx 0.25$. This value is significantly smaller than the volume quadrupole deformation, $\beta_{2,\text{U}}$, of this nucleus, and all values of $\beta_{2,\text{U}}^{\text{WS}}$ used so far in hydrodynamic calculations. The difference is a direct consequence of the sizable hexadecapole moment of ^{238}U . In what follows, we demonstrate its impact on the interpretation of high-energy data.

For ^{197}Au , we find a triaxial shape for all parametrizations, with $\gamma_{\text{Au}}^{\text{WS}} = \text{atan}(\sqrt{2}\beta_{22,\text{Au}}^{\text{WS}}/\beta_{20,\text{Au}}^{\text{WS}}) \approx 47^\circ$, agreeing with the recent MR EDF calculation [27]. The fitted WS parameters are larger than the corresponding multipole moments and can serve as an illustration that the interplay between different deformation modes is indeed nontrivial.

Understanding RHIC data.—In what follows, we restrict ourselves to the WS parameters obtained with the BSkG2 parametrization; their values, as well as those predicted by the other parametrizations, are included in Supplemental Material [41]. We now show that our analysis improves the description of elliptic flow data in $\text{U} + \text{U}$ collisions. We first go back to Eq. (1). Combining $a_0 = 25.6 \pm 5$, $a_1 = 1.18 \pm 0.05$, and $a_2 = 1.00_{-0.05}^{+0.00}$ deduced in Ref. [13] with $\beta_{2,\text{Au}}^{\text{WS}} = 0.14$ and our newly derived $\beta_{2,\text{U}}^{\text{WS}} = 0.25$ leads to $r_{\text{Au,U}}\{2\} = 1.55 \pm 0.10$, which is finally compatible with the value measured by STAR Collaboration in $\text{U} + \text{U}$ collisions at 0%–1% centrality, 1.49 ± 0.05 [1], restoring consistency between high- and low-energy nuclear phenomenology.

We demonstrate this as well in a direct model application by repeating the IP-Glasma+MUSIC+UrQMD calculations of Ref. [12], this time using the WS parametrizations of ^{238}U and ^{197}Au from the BSkG2 results (including, in addition, hard-core repulsion among nucleons [50]). We show the predicted $r_{\text{Au,U}}\{2\}^2$ in Fig. 2 as a function of collision centrality (dashed line), which is also compared to

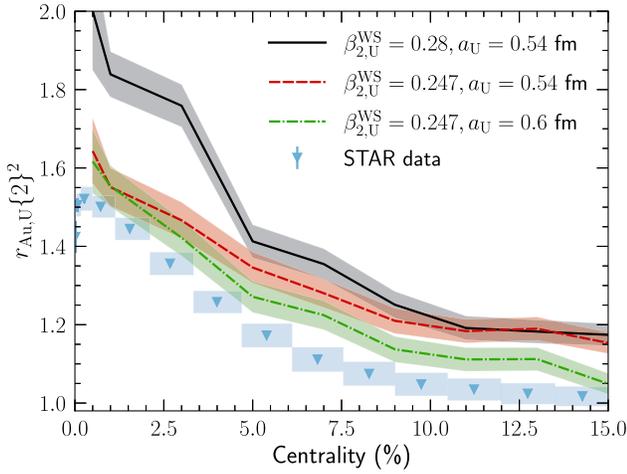


FIG. 2. Ratio of mean squared elliptic flow coefficients $v_2\{2\}^2 \equiv \langle v_2^2 \rangle$ taken between central U + U and central Au + Au collisions. Symbols: STAR Collaboration data. Lines are the results of IP + Glasma + MUSIC + UrQMD simulations. Different line styles imply different WS parametrizations for the collided nuclei. Solid line: original WS parametrizations from Refs. [11,12]. Dashed line: parametrizations from the Skyrme-EDF calculations of this manuscript. Dot-dashed line: same as the dashed line but with $a_U = 0.60$ fm.

the original predictions using $\beta_{2,U}^{WS} = 0.28$ (solid line). For 0%–1% collisions, we find that a proper implementation of the deformation of ^{238}U , obtained consistently from state-of-the-art EDF calculations, leads to results that are in agreement with both STAR data and the model-independent estimate given in Eq. (7). We have checked in addition that an initial state estimator of the shown ratio, based on eccentricities, exhibits the same behavior.

Moving away from the most central bin, we see that the description of STAR data worsens significantly. This is unlikely to be caused by the deformation parameters, but rather by an inappropriate implementation of the skin of ^{238}U in the simple WS parametrization. To show this, we repeat our calculation with a 10% larger parameter a for ^{238}U (dot-dashed line in Fig. 2). This mild correction impacts significantly the centrality dependence of $r_{\text{Au,U}}\{2\}^2$, without affecting the 0%–1% bin, corroborating the robustness of our main conclusion.

In the future, one should move away from WS densities and directly input the results of EDF calculations in hydrodynamic simulations, taking into account the difference between spatial distributions of protons and neutrons. For ^{238}U , this should be especially important due to the strong polarization of its neutron skin across the surface [53,54], whose effect in high-energy collisions may be similar to an overall broadening of the skin thickness. A recent STAR analysis of the structure of ^{238}U from ultra-peripheral collisions suggests, for instance, a larger skin than reported in common WS parametrizations [55].

Before concluding, we note that the result shown in Fig. 2 would remain unchanged if one set $\beta_{4,U}^{WS} = 0$ in the hydrodynamic simulations, as this shape parameter does not modify the eccentricity fluctuation of the QGP in central collisions [56]. A recent transport calculation [57] suggests, however, that a modest $\beta_{4,U}^{WS} \approx 0.1$ would impact the quadrangular flow v_4 , in particular, the so-called *linear* component of this coefficient in the limit of central collisions. We recommend experimental investigations of v_4 at high multiplicities and with a fine centrality binning as a potential means to independently gauge the magnitude of $\beta_{4,U}^{WS}$ at high-energy colliders.

Summary and outlook.—The difference between the deformation parameters of a WS density ($\beta_{\ell m}^{WS}$) and its multipole moments ($\beta_{\ell m}$) is particularly large when the nucleus exhibits coexisting deformation modes. ^{238}U represents such a system. Because of its sizable hexadecapole moment, the appropriate surface deformation parameter, $\beta_{2,U}^{WS} \approx 0.25$, as predicted by state-of-the-art EDF calculations with 21 different Skyrme parametrizations is significantly different from the volume deformation, $\beta_{2,U} \approx 0.28$. Past studies of relativistic U + U collisions have not accounted for this subtlety, leading to inconsistencies between BNL RHIC data and hydrodynamic calculations in central collisions. Our new simulations demonstrate that our findings resolve these issues:

$$r_{\text{Au,U}}\{2\}^2, \text{Ref. [13]} = 1.55 \pm 0.10, \quad (7)$$

$$r_{\text{Au,U}}\{2\}^2, \text{STAR data} = 1.49 \pm 0.05, \quad (8)$$

$$r_{\text{Au,U}}\{2\}^2, \text{IP-Glasma}(\beta_{2,U}^{WS}=0.25) = 1.63 \pm 0.06. \quad (9)$$

This is a major step toward establishing the consistency of theoretical and experimental results across vastly different energy scales. The preference of BNL RHIC data for values of $\beta_{2,U}^{WS}$ significantly smaller than reported in spectroscopic data tables provides evidence of the sizable hexadecapole deformation in ^{238}U , whose phenomenological consequences in high-energy collisions we have reported here for the first time.

That said, there is also some minor tension that could be addressed by the low-energy community: essentially all Skyrme parametrizations favor $\beta_{4,U}$ values that are somewhat larger than those determined from muonic x-ray and Coulex experiments, which result from model-dependent analyses. We hope that the present study will motivate future investigations of the hexadecapole moment and the $B(E4)$ g.s. transition rate of ^{238}U .

Both ^{238}U and ^{197}Au are well described by a single mean-field configuration with a well-defined shape that is reasonably consistent across models. This is not the case for all other species collided so far: for example, so-called *isobar collisions* at BNL RHIC [8] involve the transitional

isotopes ^{96}Ru and ^{96}Zr , for which a more advanced many-body treatment is required, whether based on an EDF or in an *ab initio* setup. The analysis of such collisions leads to WS shapes that combine sizable quadrupole and octupole *surface* deformation parameters [58]. In any effort from the community to confront these data with state-of-the-art calculations, corrections due to the interplay between all relevant deformation modes should be accounted for.

As anticipated, one way to achieve this is by moving away from simple shape parametrizations to generate the initial conditions for hydrodynamic simulations, sampling instead nucleon distributions directly provided by nuclear theory. Unfortunately, this does not reduce the model dependency of such analysis: predictions for the shape of nuclei may vary widely across calculations. A truly model-independent way to construct initial conditions for hydrodynamic simulations based on experimental information on nuclear multipole moments seems impossible: the $\beta_{\ell m}$ are not coefficients in a series expansion and do not uniquely characterize the nuclear density.

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