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# Unexpected Rise in Nuclear Collectivity from Short-Range Physics

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We discover a surprising relation between the collective motion of nucleons within atomic nuclei, traditionally understood to be driven by long-range correlations, and short-range nucleon-nucleon interactions. Specifically, we find that quadrupole collectivity in low-lying states of  $^6\text{Li}$  and  $^{12}\text{C}$ , calculated with state-of-the-art *ab initio* techniques, is significantly influenced by two opposing  $S$ -wave contact couplings that subtly alter the surface oscillations of one largely deformed nuclear shape, without changing that shape's overall contribution within the nucleus. The results offer new insights into the nature of emergent nuclear collectivity and its link to the underlying nucleon-nucleon interaction at short distances.

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While the emergence of dominant collective shapes in atomic nuclei from elementary particle considerations has been recently shown in large-scale *ab initio* calculations [1], how exactly the underlying physics of quarks and gluons imparts collectivity remains elusive. Nuclear collectivity is historically understood to be driven by long-range correlations that deform the nucleus; deformed nuclei can rotate, which involves all particles in the system in a correlated motion [2]. Every nucleus can take on several shapes, typically one or two [1], and the deformation of each nuclear shape is often inferred from its equilibrium “static” deformation, whereas the “snapshots” of the shape's surface dynamics are called dynamical deformation (Fig. 1). The extent of collectivity is informed by electric quadrupole moments  $Q_2$ , or equally, reduced transition strengths  $B(E2)$ , which increase with larger deformation [3]. The prevalence of large deformation in most nuclei, even those with a practically spherical ground state but with nearby well-deformed excited states [4], is now evident from the vast body of experimental data (see the reviews [5,6] and references therein). Furthermore, recent measurements of  $B(E2)$  strengths have achieved such precision that they can now test microscopic approaches and the underlying inter-nucleon forces they adopt (e.g., [7,8]).

Yet, with no available nuclear force expressed directly in quark and gluon degrees of freedom, it remains unclear which parts of such fundamental interactions are responsible for the universal preference of large deformation, and are capable of substantially influencing collectivity. Fortunately, some insight emerges when the nuclear force is modeled with the state-of-the-art chiral effective field theory (EFT) (e.g., [9–12]). Chiral EFT starts from nucleon and pion degrees of freedom, while accounting for the symmetry and symmetry-breaking patterns of the underlying theory of quantum chromodynamics (QCD). Chiral EFT hence provides a link to quark-gluon physics, which at low energies relevant to nuclei is encapsulated in its so-called low energy constants (LECs). The nuclear force thus

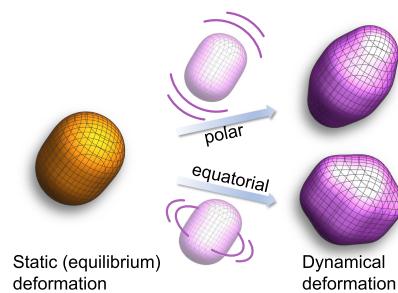


FIG. 1. Schematic illustration, based on large-scale *ab initio* calculations [1], of the static deformation (yellow) of a nuclear shape and two snapshots of its dynamical deformation (purple) arising from energetic surface oscillations (particle-hole excitations): “polar” aligned with the symmetry axis, and “equatorial” in the orthogonal plane.

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partly depends on these unknown parameters which are typically fit to experimental few-nucleon data and might eventually be informed by QCD [13–15]. In this framework, we can directly probe the response of collective observables to the physics at very short distances by varying the subset of LECs that determine the nucleon-nucleon (NN) contact interaction strengths.

In this Letter, we report on a surprising new result: that nuclear collectivity can be enhanced not only through the traditional mechanism of shapes with ever-larger deformation, but also by a spatial redistribution—mediated by the short-range  $S$ -wave NN contact interaction—of the surface oscillations of a single nuclear shape. Specifically, we discover that the LEC-independent part of the interaction, which includes the long-range one-pion-exchange force, determines the shapes and their contributions within a nuclear state, while at the same time variations of the short-range forces can further increase or decrease collectivity. The unexpected origin of this interesting effect, we find here, is subtle changes in the surface oscillations of one largely deformed and predominant shape, and the corresponding competition toward lower total kinetic energy or potential energy of the nucleus.

We examine this by providing, for the first time, response analyses of nuclear quadrupole moments, presented here for low-lying states of the odd-odd and prolate  ${}^6\text{Li}$ , and the even-even and oblate  ${}^{12}\text{C}$ , while using sensitivity analyses to detect correlations or a lack thereof among the LECs. The sensitivity calculations utilize the methodology of global sensitivity analysis (GSA) [16,17], which is often prohibitively expensive since the number of model evaluations required for convergence grows rapidly with the number of model parameters. Fortunately, the symmetry-adapted no-core shell model (SA-NCSM) [18–20] alleviates the cost of each evaluation by utilizing a fraction of ultralarge no-core shell model spaces without compromising the accuracy of the results. The SA-NCSM is an *ab initio* approach that has provided successful descriptions of electric quadrupole moments [18] and transition strengths without utilizing effective charges [7,8,21], beta decays and energy spectra [22,23], clustering features [22,24,25], and even reaction dynamics [18,26–28], up through the calcium region. It produces the same results as the traditional no-core shell model [29,30] for a given internucleon interaction, characterized by the number of harmonic oscillator (HO) shells accessible to the nucleons, and the HO intershell energy  $\hbar\Omega$ . Within this framework, we probe the response of collective features to variations in the short-distance NN coupling strengths, given by eleven LECs in chiral two-body potentials that are associated with the contact interactions of two nucleons, shedding new light on emergent collectivity in nuclei.

*Resilience of nuclear shapes*—To achieve this, we start with the  $\text{NNLO}_{\text{opt}}$  chiral NN potential [31], which is used without three-nucleon forces shown to contribute minimally

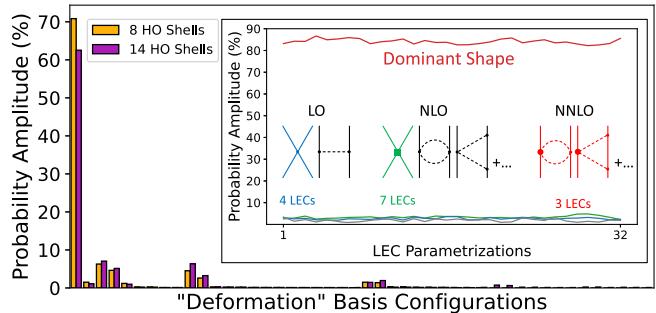


FIG. 2. Probability amplitudes of the “deformation” basis configurations of the  ${}^6\text{Li}$   $1_{\text{g.s.}}^+$  ground state calculated with  $\text{NNLO}_{\text{opt}}$  in complete model spaces of 8 (yellow) and 14 (purple) HO shells (shown are contributions with probability amplitude  $\geq 0.1\%$ ). Inset: The four nuclear shapes with the largest probability amplitudes in the 8-shell  ${}^6\text{Li}$   $1_{\text{g.s.}}^+$  state across 32 NN parametrizations uniformly sampled within  $\pm 10\%$  around the 14  $\text{NNLO}_{\text{opt}}$  coupling constants (see text for details; cf. Supplemental Material, Fig. 1 [34] for the  ${}^6\text{Li}$   $3_1^+$  state). While not shown, the inset results remain practically unchanged for 1%–50% LEC variations [42]. Also shown are the Feynman diagrams for chiral NN forces up to NNLO with the total number of LECs per order.

to three- and four-nucleon binding energies [31]. This potential is parametrized by 14 coupling constants from Feynman diagrams included up to next-to-next-to-leading order (NNLO) in the chiral expansion. Furthermore,  $\text{NNLO}_{\text{opt}}$  has been found to reproduce various observables and yield results equivalent to those obtained from chiral potentials that require three-nucleon forces, including, e.g., the  ${}^4\text{He}$  electric dipole polarizability [32] and  $A = 8$  energy spectra and quadrupole moments [22].

An NNLO chiral NN potential such as  $\text{NNLO}_{\text{opt}}$  includes the following LECs: 11 contact couplings  $C_{1S_0(pp,np,nn),3S_1}^{(\text{LO})}$  and  $C_{1S_0,3S_1,3S_1-3D_1,3P_{0,1,2},1P_1}^{(\text{NLO})}$  at next-to-leading order (NLO) for a given partial wave  $2S+1\ell_J$ , along with  $c_{1,3,4}$  at NNLO which parametrize the subleading two-pion exchange interaction (Fig. 2, inset). We note that pure  $D$ -wave contact interactions are not present as they emerge at the next chiral order (N3LO), and that by using  $\text{NNLO}_{\text{opt}}$  this Letter adopts its regulator function and cutoff. Besides the GSA, these LECs are uniformly sampled using a Latin hypercube design [33], each bounded within  $\pm 10\%$  of its  $\text{NNLO}_{\text{opt}}$  value.

First, using  $\text{NNLO}_{\text{opt}}$ , we perform SA-NCSM calculations—with no *a priori* approximations or assumptions—in the so-called “deformation” many-body basis, known as the SU(3)-adapted basis [19,43]. We use complete model spaces, that is, with all possible basis states given the number of accessible HO shells. Clearly, as shown in Fig. 2 for the  $1_{\text{g.s.}}^+$  state of  ${}^6\text{Li}$ , the probability amplitudes calculated in a model space of 8 HO shells vary only slightly compared to those calculated in the drastically

larger model space spanned by 14 HO shells. Similar outcomes are observed for excitation energies and quadrupole moments (see Fig. 4 in Supplemental Material [34]). These results indicate that the 8-shell model spaces are sufficient for our analysis that requires hundreds of thousands of large-scale computations, especially since the focus here is on responses to variations in the coupling constants and the physics that tracks with such changes. In addition, without loss of generality, our calculations use a single  $\hbar\Omega = 15$  MeV, for which the rms radii converge comparatively faster (see Ref. [1], Supplemental Material [34]).

A very interesting result emerges when we further consider the  ${}^6\text{Li}$  ground state in the so-called “shape” many-body basis, known as the physically relevant  $\text{Sp}(3, \mathbb{R})$ -adapted basis [1,18–20].  $\text{Sp}(3, \mathbb{R})$ -preserving subspaces represent microscopic nuclear shapes [3,44,45], each of which includes a static deformation and its dynamical energetic surface oscillations (Fig. 1). By “energetic oscillations” we mean multiples of  $2\hbar\Omega$  1-particle-1-hole monopole and quadrupole excitations (here, multiples of 30-MeV 1-particle-1-hole excitations), different from historically used low-energy nuclear vibrations including the so-called  $\beta$  and  $\gamma$  vibrations [2]. Remarkably, as shown in the inset of Fig. 2, the shapes—and above all the dominant shape contributing 82.2%–86.6% to the  $1_{\text{g.s.}}^+$  state—are left practically untouched across the 10% LEC variations (see Supplemental Material Fig. 1 of [34] for all the states under consideration). This implies that the one-pion and leading two-pion exchange forces, which do not depend on the 14 LECs, determine the shapes and their contributions within a nuclear state. We note that for the  $\text{NNLO}_{\text{opt}}$  parametrization, the most dominant shape comprises about 86% of the  ${}^6\text{Li}$  wave functions, whereas fourteen shapes recover about 97% of the total probabilities. In a simple picture of rigid shapes that rotate, the quadrupole moment will only vary as these probabilities vary [23,45]. Given the resilience of the nuclear shapes to LEC variations, should one then expect merely marginal effects on quadrupole moments? To answer this question, we first perform GSA on the  $Q_2$  of collective states.

*Sensitivity of collective observables*—Sensitivity analyses (e.g., [46,47]) are critical toward achieving higher-quality chiral potentials with rigorous uncertainty quantification (e.g., [42,48,49]), which, in turn, is key to advancing the frontier of nuclear large-scale simulations. Such studies further our understanding of dominant and exotic features of deformed nuclei, including clustering, octupole deformation, and nuclear properties that probe physics beyond the standard model (e.g., [50–52]). Here, in addition to reporting the first GSA for quadrupole moments, our main goal is slightly different, namely, we simultaneously vary all 14 parameters to demonstrate that  $Q_2$  is mainly sensitive to changes in the couplings individually, which allows us to independently examine different parts of the interaction.

We generate 300 000 samples in the LEC parameter space using Saltelli's procedure, implemented by the Python

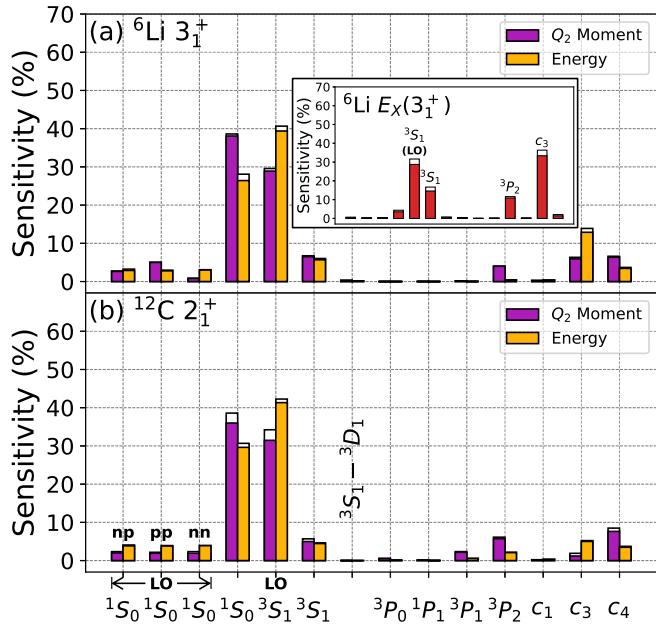


FIG. 3. First-order (colored) and total-order (white) sensitivity indices of the quadrupole moments (purple) and energies (yellow) of (a) the  ${}^6\text{Li}$   $3_1^+$  and (b)  ${}^{12}\text{C}$   $2_1^+$  states for each LEC. Calculations use SA model spaces comprised of fourteen shapes spanning 8 HO shells. Inset: Sensitivity indices for the  ${}^6\text{Li}$   $3_1^+$  excitation energy,  $E_X(3^+)$ .

library SALib [53,54]. With the aid of high-performance computing, these parametrizations are used for the state-of-the-art evaluation of 300 000 nuclear simulations—only possible in the shape basis—of the energy and  $Q_2$  moment of the  $3_1^+$  state of  $^6\text{Li}$  and of the  $2_1^+$  state of  $^{12}\text{C}$  (for the  $^6\text{Li}$   $1_{\text{g.s.}}^+$ , see Supplemental Material Fig. 2 in [34]). We find a pronounced sensitivity of  $Q_2$  to two singlet (spin-zero) and triplet (spin-one)  $S$ -wave contacts, namely,  $C_{3S_1}^{(\text{LO})}$  and  $C_{1S_0}$  (Fig. 3). This is indicated by the first-order sensitivity indices  $S_i$ , quantifying the fractional variances in the samples due to the  $i$ th coupling alone. These are the same coupling constants to which their binding energies are most sensitive, as earlier recognized in  $^{16}\text{O}$  [46], in contrast to the excitation energies (Fig. 3, inset). In addition, Ref. [55] has shown that the  $4^+$  to  $2^+$  energy ratio in selected neon and magnesium isotopes is most sensitive to the subleading singlet  $S$ -wave contact and a pion-nucleon coupling, with no dominant triplet  $S$ -wave feature.

To enable this huge number of calculations, required for convergence of the GSA results, we utilize symmetry-adapted (SA) model spaces selected from fourteen shapes spanning 8 HO shells. We find that the resulting sensitivity patterns are practically unchanged across various model space selections and sizes. We show this for  ${}^6\text{Li}$  in model spaces comprised of 1 shape, 14 shapes, and all possible shapes (corresponding to the complete model space), and in larger model spaces comprised of 10 and 12 HO shells in

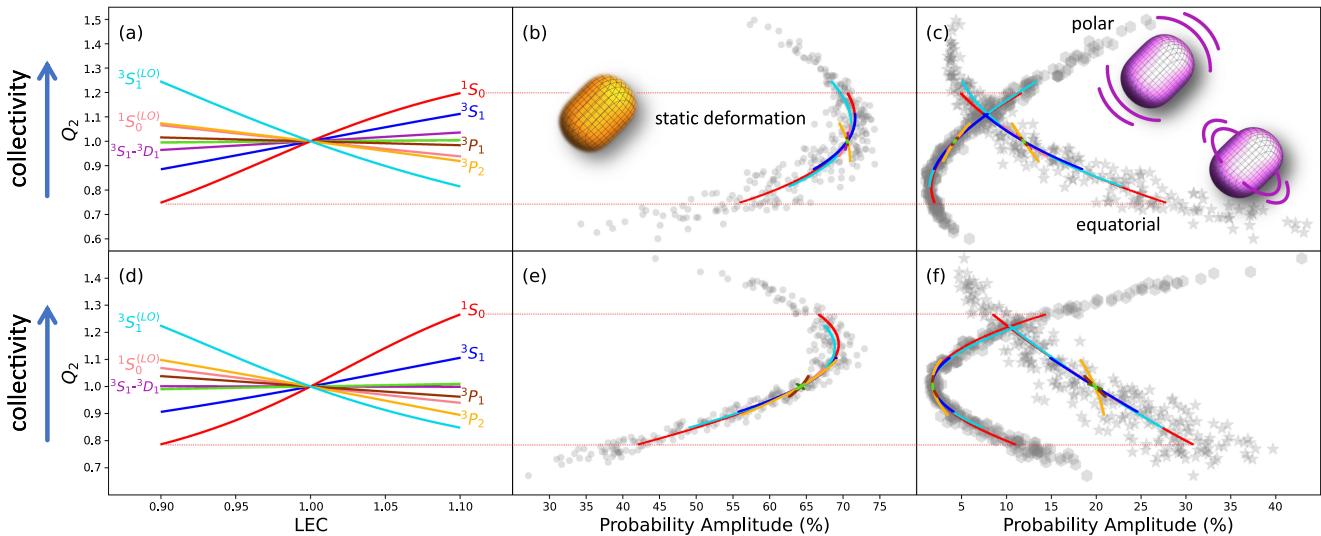


FIG. 4. Quadrupole moments  $Q_2$  relative to their NNLO<sub>opt</sub> values, of (a)–(c) the  ${}^6\text{Li}$   $3^+$  and (d)–(f)  ${}^{12}\text{C}$   $2^+$  states for each contact LEC (represented by solid curves of the same color in all plots), individually varied  $\pm 10\%$  around its NNLO<sub>opt</sub> value. For a given  $Q_2$ , or the corresponding LEC (see the dotted lines for  ${}^1\text{S}_0$  as an example), the dominant shape is decomposed into static (0p-0h) deformation in (b) and (e), and polar (equatorial) surface oscillations along (perpendicular to) the symmetry axis in (c) and (f), shown by their probability amplitudes.  $Q_2$  moments obtained from 300 samples of the 14 LECs varied simultaneously are shown in gray for the static (circles), polar (hexagons), and equatorial deformation (stars). In all plots for  ${}^6\text{Li}$ , the model space is expanded to 12 HO shells.

Supplemental Material Figs. 2 and 3 of [34], respectively. Using the same shape-selection prescription [43] and a different set of fourteen shapes, the sensitivity analysis becomes feasible for the  ${}^{12}\text{C}$   $2^+$  state. In this way, one can utilize Hamiltonian matrices in the selected shape basis of highly reduced dimensions (e.g., four orders of magnitude reduction for the  $2^+$ ) that can serve as emulators, similarly to, e.g., [56–62]. Indeed, we find that the sensitivity pattern for  ${}^{12}\text{C}$  [Fig. 3(b)] closely resembles that of  ${}^6\text{Li}$ .

Importantly, the total-order sensitivity indices, which additionally include correlations with all remaining LECs, practically coincide with the first-order indices  $S_i$  (Fig. 3). This suggests that the main effect of each coupling constant on  $Q_2$  is largely decoupled from those of the remaining parameters, and can be explored separately. This is especially useful since the sensitivity indices are normalized to the total variance of the  $Q_2$  distributions sampled, and thus provide a relative contribution to the variance, regardless whether the variance itself is small or large. The way in which each contact coupling affects the magnitude of  $Q_2$  itself can hence be understood by studying the responses of the LECs individually, as discussed next.

*Short-range footprints on long-range physics*—We find that non-negligible nuclear quadrupole moments of collective states, such as the  ${}^6\text{Li}$   $3^+$  and  ${}^{12}\text{C}$   $2^+$  states, can be enhanced by nearly 40% through the simultaneous action of two competing S-wave contact interactions, which do so via an unexpected mechanism. To show this, we first fix all coupling constants but one to their NNLO<sub>opt</sub> values, and draw 300 samples for each individual LEC, following a

Latin hypercube design (Fig. 4, where for visual clarity we exclude the LO proton-proton and neutron-neutron  ${}^1\text{S}_0$  contacts, and since we focus on the contact physics, similarly exclude  $c_1$ ,  $c_3$ , and  $c_4$ ; for completeness, we provide all these in [34]).

Corroborating the GSA results of Fig. 3 and Supplemental Material Fig. 2 [34], Fig. 4 unveils additionally interesting features, namely, that  $Q_2$  depends practically linearly on the LECs, and that the  $S$ -wave contacts act in opposition: increasing the LO  $S$ -wave couplings (especially the triplet  ${}^3\text{S}_1$ ) of the attractive delta contact interaction decreases  $Q_2$ , while increasing the coupling strength of the repulsive NLO  $S$ -wave contact (dominated by the singlet  ${}^1\text{S}_0$ ) results in larger  $Q_2$  moments. We note that the stronger the LO  ${}^3\text{S}_1$  coupling, the more bound the deuteron system is, and that an attractive delta interaction has historically been used to describe pairing. Indeed, in phenomenological nuclear models, increasing the pairing strength leads to some decrease in  $Q_2$  through the mixing of nuclear shapes [63]. Surprisingly, Fig. 4 shows such a decrease in  $Q_2$ , but with practically no change in the mixing of the nuclear shapes, as discussed above (see Supplemental Material Fig. 1 [34]; cf. Fig. 2). This suggests that another mechanism might be responsible. Given the large probability amplitudes of the dominant nuclear shapes, we explore whether the observed variances of  $Q_2$  are tied to changes within these dominant shapes. Importantly, since the total quadrupole moment is the sum of  $Q_2$  contributions from each nuclear shape (as  $Q_2$  does not couple different shapes), the component of  $Q_2$  attributed to the dominant shape not only yields

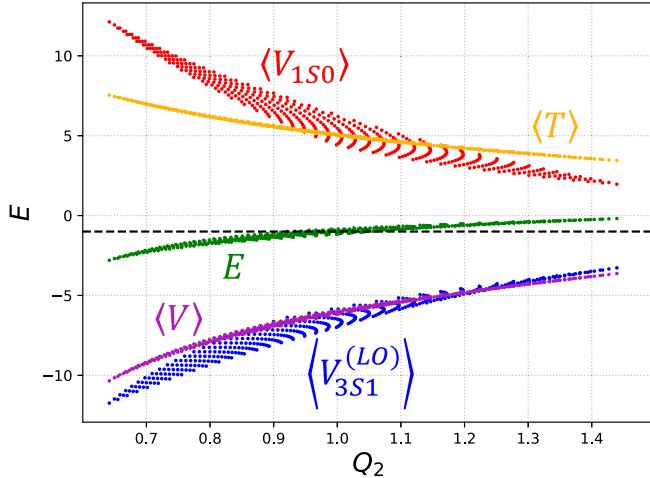


FIG. 5. The total energy  $E = \langle T + V \rangle$  of the  ${}^6\text{Li}$   $3_1^+$  state (green), the expectation value of the total potential energy  $\langle V \rangle$  (purple) and total kinetic energy  $\langle T \rangle$  (yellow), as well as of the LO  ${}^3S_1$  and NLO  ${}^1S_0$  potentials (blue and red, respectively), as functions of the electric quadrupole moment  $Q_2$ . The quadrupole moments are normalized to their NNLO<sub>opt</sub> values; the expectation values are all normalized to the absolute value of the NNLO<sub>opt</sub>  $3_1^+$  energy. Increasing  $Q_2$  values correspond to increases (decreases) in the strength of the subleading  ${}^1S_0$  (leading  ${}^3S_1$ ) LEC (Supplemental Material Fig. 6 in [34]).

most of the total  $Q_2$  value, but also exhibits nearly identical LEC dependence [e.g., for the  $1_{\text{g.s.}}^+$ , see Fig. 7(a) in the Supplemental Material [34], dashed lines].

The physics of the dominant shape unveils, for the first time, the unexpected result that the  $S$ -wave contacts of the underlying chiral potential can significantly alter the magnitude of  $Q_2$  by impacting the shape's surface dynamics: the magnitude of  $Q_2$  increases for a stronger repulsive  ${}^1S_0$  contact interaction by favoring polar oscillations, that is, multiples of two HO quanta along the symmetry axis, and decreases as the equatorial modes (having HO quanta in the plane perpendicular to the symmetry axis) become dominant with a more attractive  ${}^3S_1$  contact [Figs. 4(c) and 4(f)]. This can be understood as follows: the repulsive  ${}^1S_0$  contact, by spreading nucleons to higher HO shells, reduces Pauli-principle constraints and makes prolate configurations accessible, and these are known to have low kinetic energy [64,65], as illustrated in Fig. 5. In contrast to this, as the leading  ${}^3S_1$  coupling of the attractive delta contact increases, excitations in the equatorial plane become favorable, leading to a further decrease of the negative potential energy (Fig. 5); and while this results in larger binding energy, it comes at the expense of reduced collectivity.

These two contacts together, when varied by only 10% each, can impact  $Q_2$  by up to  $\sim 40\%$  for the  ${}^6\text{Li}$   $3_1^+$  and  ${}^{12}\text{C}$   $2_1^+$  collective states (see Fig. 5 for the  $3_1^+$  state). This is also larger compared to  $\sim 6\%-13\%$  many-body model

uncertainties (see, e.g., Fig. 4 of Supplemental Material [34] and Refs. [66,67] for the infinite-space estimates for  $Q_2$  using NNLO<sub>opt</sub> for  ${}^6\text{Li}$  and  ${}^{12}\text{C}$ ). Furthermore, the importance of the polar modes cannot be understated: whether the equilibrium deformation is prolate as in  ${}^6\text{Li}$ , or oblate as in  ${}^{12}\text{C}$ , only polar oscillations will enhance collectivity. In short, we link the impact of the short-distance contact physics on nuclear collectivity to the surface dynamics that can increase (decrease)  $Q_2$  predominantly through a stronger repulsive NLO (attractive LO)  $S$ -wave contact that favors polar (equatorial) oscillations, which lower the kinetic (potential) energy. This impact is not merely marginal, which in turn makes quadrupole moments important observables to constrain realistic nuclear forces. Furthermore, we find similar outcomes when varying the LECs of another chiral potential (NNLO<sub>sat</sub> [68]), and for the intermediate-mass triaxial nucleus of  ${}^{22}\text{Mg}$  (Fig. 5 of Supplemental Material [34]).

To summarize, we find that electric quadrupole moments of light deformed nuclei, which provide a measure of their collectivity, are affected up to about 40% when two short-range chiral NN interactions are simultaneously varied within a comparatively smaller 10% range, specifically, the opposing attractive triplet and repulsive singlet  $S$ -wave contacts. Most importantly, while historically larger  $Q_2$  moments have been associated with reduced mixing between nuclear shapes or shapes of larger deformation, here, for the first time, we show that contact interactions can significantly increase the magnitude of  $Q_2$  by subtly altering the surface dynamics of (typically) one dominant nuclear shape. We show that quadrupole collectivity is maximized by enhancing the polar surface oscillations, and this is most readily accomplished by increasing the magnitude of the subleading  ${}^1S_0$  coupling or decreasing that of the leading  ${}^3S_1$  contact, both of which lower the total kinetic energy. We have thus found a direct link between an *ab initio* description of nuclear collectivity and the short-range part of the underlying strong forces between two nucleons in contact, modeled in the chiral EFT framework, shedding new light on the emergent collectivity that dominates nuclear dynamics.

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**Data availability**—The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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