Valence Neutron-Proton Orientation in Atomic Nuclei

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Abstract

It is shown that the renormalized nuclear deformations in different mass regions can be globally scaled by two probability partition factors of Boltzmann-like distribution, which are derived from the competing valence np and like-nucleon interactions. The partition factors are simply related to the probabilities of anti-parallel and fully-aligned orientations of the angular momenta of the neutrons and protons in the valence np pairs, responsible for spherical- and deformed-shape phases, respectively. The partition factors derived from the renormalized deformations are also present in the new scaling law for the energies of the first $2^+$ states. A striking concordance between the distributions of the renormalized deformations and of the newly introduced parameter for the energies of the first $2^+$ states over the extended mass region from Ge to Cf is achieved, giving strong support to the existence of two phases: anti-aligned and fully-aligned subsets of np pairs.

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The atomic nucleus is a binary-fermion quantum many-body system. Valence neutron-proton (np) and like-nucleon (nn and pp) correlations are two fundamental ingredients in determining nuclear structure [1]. Bohr, Mottelson and Pines pointed out the like-nucleon pairing in the ground states of even-even nuclei [2], while one may expect the extreme (parallel or anti-parallel) coupling of neutron and proton angular momenta in nuclei, which is induced by the strongest residual interactions [3–5]. Thus, there should be a strong competition energy-wise between np pairs having parallel and anti-parallel coupling of the angular momenta of the involved nucleons [6, 7]. It has been long recognized that the np residual interaction is primarily responsible for configuration mixing of valence nucleons in open shells and therefore plays a key role in the onset of nuclear deformation and collectivity [8, 9]. A parameter \( P = N_nN_p/(N_n+N_p) \) has been introduced to express the average number of interactions of each valence nucleon with those of the other type, which can be related to the relative integrated strengths of np and like-nucleon pairing interactions [10]. \( N_n \) and \( N_p \) refer to the numbers of particles or holes relative to the closest shell closures [11, 12]. The \( P \) parameter provides an universal description of the nuclear structure in heavy nuclei and its evolution from spherical single-particle to deformed collective motion induced by the single-particle coherent contributions of the nucleons when the Fermi surfaces are away from the shell closures [13–17]. \( P \) is also the controlling parameter of the shape phase transitions in nuclei [1, 18]. It is worth noting that the nucleus, being a finite mesoscopic system, exhibits gradual phase transitions, unlike the infinite systems for which the changes are sharp.

As far as the anti-parallel coupling of the neutron angular momentum \( j_n \) and proton angular momentum \( j_p \) is concerned, the np interaction between non-identical orbits is shared by the \( T = 0 \) isospin-scalar and \( T = 1 \) isospin-vector channels. In modern nuclear physics, special attention has been paid to the \( T = 1 \) np pairing of nucleons occupying identical orbits [6, 7]. The multiplet subset with anti-parallel coupling corresponds to the smallest number \( 2|j_n - j_p| + 1 \) of np interactions, while the largest number \( 2(j_n + j_p) + 1 \) arises from the parallel multiplet subset. The total number of available np parallel interactions obtained by summing over all single-particle orbits in the open shells, is generally much larger than that of total np anti-parallel interactions. For sd shells, the former (latter) amounts to 63 (25). In the large \( N_nN_p \) limit, if one assume nearly-degenerate or comparable interaction energies for the configurations of parallel and anti-parallel coupling, it results in that the majority of np interactions are contained in the fully-aligned subsets.
It is well known that a $np$ pair in identical $j$ orbits can couple to angular momentum 1 or $2j$, and isospin $T = 0$ \cite{3}, satisfying thus the antisymmetry of the total wave function. The total spin in the fully-aligned configuration is $S = 1$. For neutron and proton occupying non-identical orbits, the fully-aligned configuration is different. The single-particle orbits can be divided into two categories depending on the spin-orbit $ls$ coupling. Let $j_> = l + 1/2$ and $j<_{} = l - 1/2$ denote the angular momenta resulting from parallel and anti-parallel $ls$ couplings, respectively. If both neutron and proton occupy the non-identical $j_>$ orbits, the spin of the fully-aligned configuration is $S = 1$. The antisymmetry of the total $np$ wave function leads to a relatively pure $T = 0$ $np$ pair. Here we adopt the principle that the central force dominates the nuclear force and requires the spatial symmetry. For the other combinations, the fully-aligned state includes $T = 0$ and $T = 1$ components. Taking into account that the majority of $np$ interactions come from the fully-aligned states and the $T = 0$ interaction is stronger, we can therefore infer the existence of a $T = 0$ condensate of $np$ pairs in the large $N_nN_p$ limit. However, the probability partition between the two kinds of extreme coupling has so far been missing. In this Letter, we present for the first time the probabilities of anti-aligned and fully-aligned subsets of $np$ pairs in nuclei.

It is the fully-aligned subset of $np$ pairs that plays the most important role in the onset of deformation and collective rotational motion, as discussed earlier in Refs. \cite{19,20}, but without mentioning the $np$ pairs. Danos and Gillet therefore introduced a concept of two identical chains consisting of fully-aligned $np$ pairs for $N = Z$ even-even nuclei to interpret the collective rotation as the gradual alignment of the paired chains \cite{21,22}. They are called Ising-like chains hereafter because the $np$ angular momentum is an analogue of the Ising spin residing on the Ising chain \cite{18,23}. The absence of deformation and anti-parallel $np$ pairs in the Ising-like chains discussed by Danos and Gillet \cite{21,22} for $N = Z$ nuclei, makes the chains imperfect and unrealistic when applied to real nuclei. We extend here the Ising concept to $N \neq Z$ cases, also including the anti-parallel $np$ pairs. An even-even nucleus is composed of $N_n/2$ valence-neutron and $N_p/2$ valence-proton pairs. $N_n/2$ neutrons and $N_p/2$ protons can be picked out from the like-nucleon pairs to form $\sqrt{N_nN_p}/2$ effective $np$ pairs despite the fact that non-integer values are obtained for unequal numbers of valence neutrons and protons. The $np$ pairs with two kinds of extreme (anti-parallel and fully-aligned) coupling are the building blocks of a macroscopic chain carrying a spin $J_{np}$ which can vary between a minimum ($J_{np}^{\text{min}}$) and maximum ($J_{np}^{\text{max}}$), following an unknown distribution with some
probability. The remaining nucleons not involved in the construction of Ising-like chain, constitute the other macroscopic twin chain having opposite spin. The two Ising-like chains are paired in the ground state and the spins of the constituents gradually align along the rotation axis for rotation motion.

The total number of effective $np$ pairs which is $2\sqrt{N_nN_p}/2 = \sqrt{N_nN_p}$ for two Ising-like chains, results from the number $N_nN_p$ of $np$ pairs formed by $N_n$ neutrons and $N_p$ protons and the synthesis probability of a $np$ pair. Since the probability of selection of a neutron and a proton from $N_n/2$ pairs of neutrons and $N_p/2$ pairs of protons is $1/N_n$ and $1/N_p$, respectively, the synthesis probability of a $np$ pair is defined as the overlap of the wave functions of a neutron and a proton [24, 25], normalized to the respective square root of selection probabilities $\sqrt{1/N_n}$ and $\sqrt{1/N_p}$, which is $1/\sqrt{N_nN_p}$. One can verify that for $N_n = N_p$, the number $\sqrt{N_nN_p}$ of effective $np$ pairs becomes $N_n$ or $N_p$, which shows that the proposed extension of the Ising concept to $N \neq Z$ cases is coherent.

One generally believe that the configuration mixing is responsible for deformation [9]. It is certainly true for the Ising-like chains. The mixing is achieved in a series of chains with spins $J_{np} \otimes J_{np} = J \otimes J, (J-1) \otimes (J-1), (J-2) \otimes (J-2), \cdots$, where $2J$ represents the nuclear total angular momentum. The mixing mechanism is similar to that generated by the quadrupole field $r^2 Y_{20} \sim z^2 - x^2 \sim r(z - x)$ acting on a single-particle, which mixes the unique-parity Nilsson orbits [26]. As for the macroscopic chains, the difference $R_z - R_x$ contained in the whole quadrupole operator $R^2 Y_{20}$ is effective in inducing the mixing, which accounts for the deformation mechanism of Ising-like chains in the framework of the spherical shell model [9]. The Ising-like chains therefore bridge the spherical and deformed shell models [26–31]. The axially symmetric quadrupole deformation is related to the asymmetry of the long and short axes through the parameter $\beta \sim (R_z - R_x)/(1.2A^{1/3})$, which is positive for prolate ($R_z > R_x$) and negative for oblate ($R_z < R_x$) shapes. We realize that the renormalized shape parameter $\beta A^{1/3}$ is a measure of the extent of effective quadrupole mixing of Ising-like chains and might be considered as a global observable over the entire nuclear mass table.

Much effort has been devoted to the regional systematics of the quadrupole deformation parameter $\beta$ of the even-even isotopes from Germanium to Californium, the regions being divided by closed shells or sub-shells [32–36]. The present study, which employs the renormalized deformation $\beta A^{1/3}$, goes beyond the systematics over limited mass regions. We employ the correlation scheme of the renormalized deformation $\beta A^{1/3}$ and $P$ factor to
FIG. 1. (Color online) $\beta$ vs $P$ for (a) Polonium-Californium isotopes; (b) Strontium-Cadmium isotopes with $N > 50$. Note that the enclosed Po isotopes deviate from the systematics because of their neutron numbers less than the magic number 126. Zr-Mo (Sr) isotopes undergo a sharp change of shape at $N = 60$ due to the collapse of proton sub-shell closure 38 and the creation of sufficient valence space for deformation and the closed shell $Z = 50$ (28) has to be used as the new reference core. The deviation of $\beta$ values of $^{92-96}$Zr is due to the proton sub-shell closure 40 resulting in the effective $N_p = 0$ rather than 2 relative to 38, which are omitted in the following figures.

examine the independence and judge the adequacy of the description employing Ising-like chains. All the data are taken from the recently compiled Table 3 in Ref. [36].

Nuclear deformations in different mass regions always show a rise until saturation for nuclei with mass number $A > 150$, after undergoing an inflection at a certain $P_c$ value. Two typical examples are shown in Fig. 1 for Strontium-Cadmium and Polonium-Californium isotopes. The overall growth of the deformation can be easily understood as induced by the enlarged $np$ interaction energy which increases with increasing $N_n N_p$, while the saturation can be attributed to the attenuation of the interaction between valence neutrons and protons near mid-shells occupying extremely different orbits [37, 38]. However, it is obviously questionable whether the saturation exists in any light-mass region. Comparing the resemblance or difference of such plots with those of a complete set covering several regions would contribute to solve the problem.

It is well known that the nuclear deformations show an overall decrease from the lightest to heaviest nuclei [36]. The initial $\beta$ value of $A \sim 110$ nuclei tends to be 0.07 larger than that
FIG. 2. (Color online) Renormalized $\beta A^{1/3}$ vs $P - P_c$ for the ground state of even-even nuclei: Po-Cf (black), Dy-Hg (red), Te-Gd with $N > 82$ (blue), Te-Gd with $N < 82$ (yellow), Kr-Cd with $N > 50$ (pink), and Ge-Zr with $N < 50$ (green), where $P_c$ is taken from Table I. Ce-Dy (Er-Hf) isotopes undergo a sharp change in the shape and excitation energy at $N = 88$ due to the collapse of proton sub-shell closure 64 and the closed shell $Z = 50$ (82) has to be used as the new reference core. We propose two identical Ising-like chains consisting of parallel or fully-aligned $np$ pairs for simplicity responsible for the unification of nuclear spherical single-particle and deformed collective properties as $P - P_c$ going from the negative to positive infinite limits corresponding to the infinite limits of valence-nucleon numbers.

of $A \sim 220$ nuclei, while one expects an increase of $\beta$ by a factor of near two for $P = 6$ (see Fig. 1). Taking into account the dependence of $\beta$ on the asymmetry of the nuclear radius $\beta \sim (R_x - R_z)/(1.2A^{1/3})$, the decrease of the deformation $\beta$ with increasing $A$ should be associated with the $A^{-1/3}$ dependence [36]. We found that the renormalized deformations, independent of the mass region, are universally valid around their inflection $P_c$ parameters given in Table I. A similar universality is also present for the excitation energies, around the same $P_c$ values (see the following discussion). Figure 2 shows that the renormalized

TABLE I. Inflection $P_c$ values of the $P$ parameter and saturated energy ratios $R_s$ for given mass regions.

| Region    | Po-Cf | Dy-Hg | Te-Gd (N>82) | Te-Gd (N<82) | Kr-Cd (N>50) | Ge-Zr (N<50) |
|-----------|-------|-------|--------------|--------------|--------------|--------------|
| $P_c$     | 3.53  | 4.6   | 3.6          | 4.45         | 4.6          | 4.75         |
| $R_s$     | 32.78 | 16.00 | 17.16        | 12.94        | 12.70        | 10.86        |
FIG. 3. (Color online) Renormalized $2^+_1$ energy ratio $R$ of the single closed-shell nucleus to its isotope being studied vs $P - P_c$: Po-Cf (black), Dy-Hg (red), Te-Gd with $N > 82$ (blue), Te-Gd with $N < 82$ (yellow), Kr-Cd with $N > 50$ (pink), and Ge-Zr with $N < 50$ (green), where the saturated energy ratio $R_s$ is taken from Table I. The following replacements of $2^+_1$ energies of single closed-shell nuclei by those in the nearest available neighbors have been made for the lack of excitation energies. $^{216}$Th has been tentatively utilized to replace U-Cf isotopes with $N = 126$. We use the $^{134}$Te ($^{98}$Cd) to replace the single closed-shell nuclei of Ce-Hf (Sr-Mo) isotopes at $N \geq 88$ (60). $^{154}$Hf has been used to replace the single closed-shell nuclei of W-Hg isotopes as $N_n < 16$; $^{206}$Hg has been used to replace the single closed-shell nuclei of W-Hf isotopes as $N_n \geq 16$ (the sudden change of excitation energy at 16 rather than midshell 22). $^{128}$Pd has been used to replace $^{126}$Ru for Ru isotopes.

deformations of nuclei in different mass regions fall into a twisted band centered around the $P - P_c = 0$ inflection point. A striking regularity is therefore achieved. A curve drawn through the center of the band tends to start from $\frac{\beta A^{1/3}}{3} \approx 0$ and terminate at $\frac{\beta A^{1/3}}{3} \approx 2$.

A step function with four parameters has been employed to well reproduce the reduced transition probabilities of actinides in Ref. [34]. The curve drawn in the $\beta A^{1/3} \ vs \ (P - P_c)$ plot appears to have a similar form, but needs only two parameters, $\lambda$ and $P_c$. A universal scaling law is therefore adopted for the renormalized deformations in the form

$$\beta A^{1/3} \approx 1 + \tanh[\lambda(P - P_c)],$$

where $\tanh$ is the hyperbolic tangent function, and the constant $\lambda = 0.3135$. The function contains two probability partition factors $e^{\lambda(P - P_c)}$ and $e^{-\lambda(P - P_c)}$ of a Boltzmann-like distribution because the variation of $\beta A^{1/3}$ in the interval 0 to 2 can be obtained with a $2e^{\lambda(P - P_c)}/[e^{\lambda(P - P_c)} + e^{-\lambda(P - P_c)}]$ statistical weight. The parameter $\lambda P$ is the analog of $E/kT$. 

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of the Boltzmann distribution. In the limit of an infinite system, the universal form obviously indicates spherical- and deformed-shape phases [1, 18]. The two phases can attain the equilibrium at the inflection point, called critical point henceforth. Coexistence of deformed and spherical shapes, as well as fairly similar order parameters, are expected for nuclei around a given point on the curve.

The most distinctive feature of the scaling law for nuclear shape is the unification, which reveals a general Boltzmann-like distribution for even-even nuclei from Germanium to Californium, emerging from the interplay of the np interaction and like-nucleon pairing correlations. Note that it is a quantum-mechanical behavior essentially different from the Boltzmann thermodynamic one. It can be shown that the correlation energy $E$ of $N$ Ising spins [23] abiding by a Boltzmann distribution is proportional to $N^2$ (see Eq. 1.12 in Ref. [18]). In the case of the nuclear system, there is also a quadratic dependence of the number of involved nucleons with the form $N_n N_p$, which enter in the expression of the correlation energy. The appearance of the $N_n N_p$ product in the Boltzmann-like distribution offers the possibility of reinterpreting its physical significance as a measure of the correlations embedded in the constituent $\sqrt{N_n N_p}$ effective np pairs.

For nuclei near the closed shells, the valence neutrons and protons tend to align antiparallel to maximize the np residual interaction [3–5] and any two neighboring np pairs along a chain are expected to be paired to spin zero along a chain [2]. The resultant chain carries a minimum spin near $J_{np}^{min} = 0$. For nuclei near the mid-shells, parallel orientation is favored in energy for neutrons and protons in np pairs. This is because the anti-parallel states are already filled and the interaction in the fully-aligned configuration is usually the second strongest [3–5]. Furthermore, long-range correlations dominated by the quadrupole and octupole components [39] exist between any two np pairs along a chain, which may overcome the short-range pairing correlations occurring only between the neighboring np pairs and two Ising-like chains. The long-range correlations therefore result in the parallel orientation of np pairs. The resultant chain carries a maximal spin.

In the limit of infinite number of valence nucleons, the angular momenta of the neighboring neutron and proton along a chain [21, 22] are expected to be completely antiparallel (lower chains in Fig. 2) and parallel (upper chains in Fig. 2) for spherical- and deformed-shape phases, respectively. In a general state, np pairs with parallel orientation of the neutron and proton angular momenta are present in the deformed phase with its statistical
weight $e^{\lambda(P-P_c)}/[e^{\lambda(P-P_c)} + e^{-\lambda(P-P_c)}]$, coexisting with $np$ pairs having anti-parallel orientation of the neutron and proton angular momenta in the spherical single-particle phase. The deformation of the nucleus in a general state results from the mixing of the spherical- and deformed-shape phases, and finally relies only on the $\beta$ of the latter and its statistical weight, since the deformation $\beta$ of the spherical-shape phase is zero.

The probability of parallel orientation of the angular momenta of the neutron and proton in the valence $np$ pairs is small when $P$ is close to zero, reaches up to 0.5 at $P = P_c$, and tends to the maximum value of 1 in the limit of large $P$. Accordingly, the deformation undergoes the slow-steep rise up to the critical point, and thereafter gradually gets saturated. The pairing correlations show an overall decrease from the lightest to heaviest nuclei. The pairing correlations lead the $np$ pairs easy and hard to step into the phase of parallel alignment of the angular momenta of the neutron and proton for heavy and light nuclei, respectively. This reveals the significance of the overall decrease of the critical point from the light to heavy regions in Table I except for the obvious deviation in the Dy-Hg region, where the valence nucleons occupy the orbits with the highest $j$ in the proton and neutron shells, $\pi h_{11/2}$ and $\nu i_{13/2}$, leading to an enhancement of the $j$-dependent pairing forces.

After gaining an insight into the orientation of the angular momenta of the valence neutrons and protons in the $np$ pairs, we proceed to the two-body correlations between $np$ pairs. The excitation energy $E_{2^+}$ of the first $2^+$ state as the result of two-body correlations is another typical example of the indicator of single-particle or collective degrees of freedom decreasing along its isotopic chain from the single closed-shell nucleus to a near-constant value for the mid-shell nuclei. Let $R$ denote the ratio between $E_{2^+}$ of a single closed-shell nucleus and that of a given isotope. The quantity $R$ varies regularly from unity to a value $R_s$ close to saturation. The adopted $R_s$ values for different regions are given in Table I. We define a new parameter $O = (R - 1)/(R_s - 1)$ and found that it is universally valid, independent of the mass region, around the same critical points as the renormalized deformations. Figure 8 shows that the renormalized energy ratios are confined in a band similar to that in Fig. 2 by using the same critical points (a multiplicative factor of 2 in the numerator is employed to allow the comparison with Fig. 2). However, both the rise and saturation are more rapid. A function similar to that used to fit the renormalized deformations $\beta A^{1/3}$ has been used to fit the renormalized energy ratios, in which the exponent in the hyperbolic tangent function is two times larger.
We initially speculated that the behavior of the parameter $O$ depends on $e^{2\lambda(P-P_c)}/[e^{\lambda(P-P_c)} + e^{-\lambda(P-P_c)}]^2$, because $E_{2^+}$ varies inversely proportional to $\beta^2$ [32], and $\beta$ has a variation governed by the hyperbolic tangent function involved in the scaling law of Eq. 1. The final form obtained from the fit of the experimental data differs from this general expectation. A possible reason is that we ignore the contribution of its supplement $e^{-2\lambda(P-P_c)}/[e^{\lambda(P-P_c)} + e^{-\lambda(P-P_c)}]^2$ present in the spherical-shape phase, leading to a normalized coefficient $e^{2\lambda(P-P_c)}/[e^{\lambda(P-P_c)} + e^{-\lambda(P-P_c)}]^2 + e^{-2\lambda(P-P_c)}/[e^{\lambda(P-P_c)} + e^{-\lambda(P-P_c)}]^2$. Once the $R = 1$, $O = 0$ normalization point for the spherical-shape phase is adopted, the final form including $e^{-2\lambda(P-P_c)}$ and $e^{2\lambda(P-P_c)}$ can be obtained, attesting the coexistence of two phases in the distribution of the $E_{2^+}$ energies.

In contrast with the critical point, the saturation values $R_s$ of the energy ratio parameter $O$ given in Table I show a trend which is opposite to that of the critical point parameters $P_c$. Again, the value for the Dy-Hg region is obviously abnormal. In order to understand the trend and anomaly, the analysis of the energy ratio $R$ can help. The $np$ interaction energy can be considered to cause the decrease of $E_{2^+}$ (namely increase of $R$ until saturation) from a single closed-shell nucleus towards the mid-shell nuclei [8]. Thus, the increasing trend of the saturated energy ratio $R_s$ in Table I actually reflects the saturation of the $np$ interaction for high $P$ values in heavy nuclei, while the opposite decreasing trend of the $P_c$ values as mentioned above is caused by the pairing correlations.

To summarize, we have shown that hundreds of available nuclear shapes can be encompassed in a twisted band by fixing the newly-proposed critical points. The universal form can be well scaled by a function including the hyperbolic tangent, composed of two probability partition factors of Boltzmann-like distribution for spherical- and deformed-shape phases in the limit of an infinite system, which attain the probability equilibrium at the critical points. The fraction in the probability partition factors of Boltzmann-like distribution serving as an analogue to the Boltzmann exponent manifests itself by the presence of the $np$ interaction between $np$ pairs to like-nucleon pairing correlations. Excitation energies of the first $2^+$ states exhibit the same critical points, but quadratic dependence on partition factors. The Boltzmann-like distribution of nuclear deformations is further confirmed by the excitation energies of the first $2^+$ states. We deduce that the partition factors are related to $np$ anti-parallel and fully-aligned oriented probabilities responsible for spherical- and deformed-shape phases, respectively.
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