Cluster interpretation of parity splitting in alternating parity bands

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Abstract

The parity splitting in actinides is described with a cluster model of oscillations in mass asymmetry coordinate. The spin dependence of the calculated parity splitting is in a good agreement with the experimental data.

The observation of low-lying negative-parity states near the ground state have shown that many actinides isotopes have reflection-asymmetric shapes [1,2]. However, in these nuclei the positive and negative parity states being considered together do not form undisturbed rotational bands as in the case of the asymmetric molecules. At small spins $I$ the negative parity states are shifted up with respect to the positive parity states. This shift (parity splitting) decreases with increasing $I$ and disappears at some value of spin which varies from nucleus to nucleus, although in several nuclei small oscillations of the parity splitting around zero are observed for large $I$ [3]. Thus, in contrast to molecules, in nuclei the potential barrier between a shape with reflection asymmetric deformation and its mirror image, if existing, is not large enough to prevent a barrier penetration. The penetration through this barrier lowers the energies of levels with even $I$ with respect to the energies of levels with odd $I$. However, with increasing spin the barrier becomes higher and the penetration probability goes to zero. Then we find almost ideal alternating parity bands.

Thus, there are two experimental characteristics of the alternating parity bands which should be explained: the parity splitting at the beginning of the rotational band and the critical value of spin at which the parity splitting disappears.

It was recognized that low-lying negative-parity states can be described by an octupole or dipole degree of freedom, and many studies have explored this possibility. The parity splitting related to octupole deformation was treated in Refs. [4,5] within the self-consistent microscopic model with parity projection. Phenomenological interpretation of the spin dependence of the parity splitting was realized in [6,7] where
the suggested simple exponential formula with two parameters describes the experimental data quite well. However, the parameters vary significantly from isotope to isotope and we need a nuclear structure model to understand these variations.

The aim of the present Letter is a formulation of a quite simple model which provides a quantitative explanation of the variations from nucleus to nucleus of the observed values of the parity splitting at the beginning of the rotational bands and the critical angular momentum at which the parity splitting disappears. It is shown below that collective oscillations of a nuclear shape, which lead to the formation of cluster-type shapes, explain the observed properties of the parity splitting in actinides.

The idea that alpha clustering [8–10] explains an appearance of low lying negative parity states in actinides was explored in Ref. [11] within a phenomenological model based on group theoretical methods. In [11,12] nuclear ground states correspond to dipole vibrations rather than to rigid molecular-like dipole deformations. Corresponding wave functions consist of α-cluster and mononucleus components. In contrast to this approach a cluster configuration with fixed mass asymmetry is proposed in [13] to describe the properties of the low-lying positive and negative parity states in actinides. The cluster heavier than α-cluster is taken in [13] as a light cluster.

The nuclear systems consisting of a light cluster \( A_2 \) plus a heavy cluster \( A_1 \) belong to the class of dinuclear-type shapes. They were first introduced to explain data on deep inelastic and fusion reactions with heavy ions [14]. Instead of the parameterization of the nuclear shape in terms of quadrupole \((β_2)\), octupole \((β_3)\) and higher multipole deformations, the mass asymmetry \( η = (A_1 - A_2)/(A_1 + A_2), (η = 1 \text{ if } A_2 = 0 \text{ and } A_1 = A) \) and the distance \( R \) between the centers of clusters are used as relevant collective variables [15]. Since \( η \) is a dynamical variable, the ground state wave function is a superposition of different cluster-type configurations including the mononucleus configuration with \( |η| = 1 \). In the present Letter we consider a motion in \( η \) which leads to an appearance of different cluster states and a mononucleus configuration with certain probability. The relative contributions of each cluster component in the total wave function are determined by the potential energy of the collective Hamiltonian described below. Our calculations have shown that in the considered cases the dinuclear configuration \( (η = η_0) A/Z \rightarrow (A-4)(Z-2) + {^4}\text{He} \) with an alpha cluster has a potential energy which is close or even smaller than the energy of the mononucleus at \(|η| = 1 \) [16]. Since the energies of the configurations with a light cluster heavier than an α-particle increase rapidly with decreasing \(|η|\), we can restrict our investigations to configurations with light clusters not heavier than Li \((η = η_{Li})\), i.e., to cluster configurations near \(|η| = 1 \) and not too high spins. For large angular momenta, the other cluster configurations can be also important for treating the oscillations in \( η \). The symmetric cluster configurations with \( η ≈ 0 \) have a relatively low potential energy as well. However, these configurations are characterized by very large quadrupole deformations and rather correspond to hyperdeformed states [16]. They are separated from the mononucleus configuration by a large barrier.

The potential energy of the DNS is expressed as

\[
U(R, η, I) = B_1(η) + B_2(η) + V(R, η, I),
\]

where \( B_1 \) and \( B_2 \) are the experimental binding energies of the DNS nuclei at a given mass asymmetry \( η \). Shell effects and pairing correlations are included in these binding energies. It is known [17,18] that there is a strong correlation between the setting in of an octupole deformation and the quenching of the pairing correlations. However, the pairing interaction between the nucleons of different clusters is not taken into consideration because the pairing interaction matrix elements are rather small for touching clusters. The quantity \( V(R, η, I) \) in (1) is the nucleus–nucleus potential. It is given as \( V(R, η, I) = V_{\text{coulal}}(R, η) + V_{\text{coul}}(R, η, I) + V_{\text{centf}}(R, η, I) \) with the Coulomb \( V_{\text{coul}} \), centrifugal \( V_{\text{centf}} = h^2 I(I + 1)/(2\gamma(η, R)) \) and nuclear interaction \( V_N \) potentials. The nuclear potential \( V_N \) can be obtained by averaging the nucleon–nucleon interaction over the generator coordinate (GC) wave function of a system of two clusters. The distance \( R \) plays the role of a generator coordinate and the potential is given by the diagonal part of a corresponding integral kernel of the GC method. The \( 0^+ \) ground state wave functions are taken as the cluster wave functions. In fact, only the direct part of the integral GCM kernel which neglects antisymmetrization effects is taken into account and as a consequence a double folding form of the potential \( V_N \) with the ground state nuclear densities is obtained. Antisymmetrization between nucleons
belonging to different clusters is imitated by a density dependence of the nucleon–nucleon forces which is responsible for the repulsive core in the cluster–cluster interaction potential. This density dependence describes a change in the nucleon–nucleon interaction from an attraction in the region of low nuclear density to a repulsion when the nuclear density is sufficiently large, thus taking into account the effect of the Pauli exclusion principle. Details of calculations of $V_N$ are given in [19]. The parameters of the nucleon–nucleon interaction are fixed in the nuclear structure calculations [20]. The nucleon density distribution is approximated by the Fermi distribution with the radius parameter $r_0 = 1.15$ fm. While the diffuseness parameter $a$ for $^4$He and $^7$Li is taken as 0.48 fm (in Ref. [16] (see Fig. 5 of [16]) we used 0.55 fm for all $\eta$ that is too large for $|\eta| > 0.85$ and produces too small potential energy at $|\eta| = |\eta_{\alpha}|$, we set $a = 0.56 \sqrt{B_n^{(0)}/B_n}$ fm for heavy nuclei, where $B_n$ and $B_n^{(0)}$ are the neutron binding energies of the studied nucleus and of the heaviest isotope considered for the same element, respectively.

For example, in the case of Ra, Th and U isotopes, $B_n^{(0)}$ corresponds to $^{226}$Ra, $^{232}$Th and $^{238}$U, respectively.

The potential taken as a function of $R$ has a pocket and the DNS is localized in the minimum of this pocket at $R = R_m$ corresponding to the touching configuration with a possible deformation of the heavy cluster whose characteristics are taken from [21]. The relative orientation of the deformed nuclei in the DNS follows the minimum of the potential energy which corresponds to the pole-to-pole orientation.

The nucleus–nucleus potential $V(R, \eta, I)$ and potential $U$ ("driving potential") were successfully applied to the analysis of the experimental data on fusion and deep inelastic reactions with heavy ions [22,23].

In Ref. [13] the cluster configuration with a lighter cluster heavier than $^4$He is determined as the most important one by the "maximum stability condition" which selects the configurations with the largest deviation of $B_1 + B_3$ from the corresponding liquid drop value. Since in our treatment the overlap of clusters is much smaller than in the model given in [13], the choice of relevant cluster configuration follows the minimum of the driving potential $U$, i.e., the interaction $V(R, \eta, I)$ is taken in (1) into account. As a result we describe the same nuclear properties as in [13] with cluster configurations having larger $|\eta|$ but smaller overlap of the clusters.

To calculate the potential energy at $I \neq 0$, the moment of inertia $\mathcal{I}(\eta, R_m)$ for the cluster systems has to be defined. It is known that the moments of inertia of superdeformed states are about 85% of the rigid-body limit [24]. As was shown in [16], the highly deformed states are well described as cluster systems. Therefore, we assume that the moment of inertia of cluster configurations with $\alpha$ and Li as light clusters is described by the expression

$$\mathcal{I}(\eta) = c_1 \left( \mathcal{I}_1 + \mathcal{I}_2 + m_0 A_1 A_2/R_m^2 \right).$$  \hspace{1cm} (2)

Here, $\mathcal{I}_i$ ($i = 1, 2$) are the rigid body moments of inertia for the nuclei constituting the DNS, $c_1 = 0.85$ for all considered nuclei and $m_0$ is the nucleon mass.

For $|\eta| = 1$, the value of the moment of inertia is not known from the data because the experimental moment of inertia takes intermediate value between those for the mononucleus (|\eta| = 1) and for cluster configurations arising due to the oscillations in $\eta$. We parameterize $\mathcal{I}(|\eta| = 1)$ as

$$\mathcal{I}(|\eta| = 1) = c_2 \mathcal{I}^r,$$  \hspace{1cm} (3)

where $\mathcal{I}^r$ is the rigid body moment of inertia of the mononucleus calculated with deformation parameters [21] and $c_2$ is a scaling parameter which is fixed to describe the energy of the first $2^+$ state (it can be done also for any other even parity state). The chosen values of $c_2$ vary in the small interval $0.1 < c_2 < 0.3$. So, in our calculations there is a single free parameter which is used to fit the energies of one of the known rotational states. It should be noted that the rotational states of the alternating parity bands are characterized by the energies of the positive parity states and the angular momentum dependence of the parity splitting. Our aim is a description of the parity splitting characteristics only. However, the parameter $c_2$ is used to describe the gross behavior of the rotational band. In $^{220,222,224,226}$Ra isotopes $\mathcal{I}(|\eta| = 1) = 12, 17, 22$ and $32$ h$^2$/MeV, respectively.

In $^{222,224,226,230,232}$Th isotopes $\mathcal{I}(|\eta| = 1) = 12, 20, 30, 48, 52$ and $55$ h$^2$/MeV, respectively. In the considered U isotopes $\mathcal{I}(|\eta| = 1) \approx 56$ h$^2$/MeV. Usually, the pairing interaction is important for a correct description of the moment of inertia of the mononucleus. However, in our calculations this moment of
inertia is a single parameter fixed to describe the energy of one of the experimental rotational even parity states. Note that the angular momentum is treated in this Letter very roughly. We assume that it consists of two parts, of the angular momentum of the collective rotation of a heavy cluster and of the orbital momentum of the relative motion of two clusters. Single particle effects are neglected. In principle, alignment of the single-particle angular momentum can produce a mixing of $K^\pi = 0^-$ state considered in this Letter with $K^\pi = 1^-, 2^-, 3^-$ states.

Determining the potential energy (1), we substitute the experimental masses of the clusters and calculate their nuclear and Coulomb interactions. A specific point is $|\eta| = 1$. Since the ground state wave function is distributed in $\eta$, the potential energy at $|\eta| = 1$ is fixed so as to reproduce the experimental binding energy of the $Z_A$ nucleus with respect to $U(\eta_\alpha)$. We vary the value of $U$ at $|\eta| = 1$ and solve the Schrödinger equation for $\eta$-motion up to the moment when the experimental value of the ground state energy is obtained. If the potential energy of the $\alpha$-cluster configuration is smaller than the experimental binding energy in the ground state like in $^{220, 224, 226}$Th and $^{220, 222, 224, 226}$Ra, then the potential has a minimum at $|\eta| = 1$. In the other cases the potential has a minimum at $|\eta| = 1$.

In order to solve the Schrödinger equation in $\eta$, a smooth parameterization of the potential

$$U(x, I) = U(x_\alpha, I) + \sum_{k=1}^{4} a_{2k}(I) \left( x_{2k} - x_{2k}^{\alpha} \right),$$

where

$$x = -\eta + 1 \quad \text{if } \eta > 0,$$

$$x = -\eta - 1 \quad \text{if } \eta \leq 0,$$

(4)

is used which goes through the calculated values of the potential energy at $|\eta| = 1$, $\eta = \eta_\alpha$ and $\eta = \eta_Li$. The calculations with other parameterizations show almost no difference in the description of parity splitting in the considered nuclei. If the minimum of the potential is located at $\eta = \eta_\alpha$, three parameters $a_2$, $a_4$ and $a_6$ are determined so as to fix the position of the minimum at the right place, to get correct values of $U$ for a cluster configuration with Li as the light cluster and to fix the ground state energy, which we obtain after solving the Schrödinger equation, at the right position with respect to $U(\eta_\alpha)$. The fourth parameter $a_8$ is necessary to avoid a fall down of the potential $U$ when $|\eta| \leq \eta_Li$, which appears because of the negative value of $a_6$ needed to describe correctly $U(\eta_Li)$. Since this fall down of $U$ can influence our calculations, we take the minimal necessary positive value of $a_8$ to guarantee an increase of $U$ for $|\eta| \leq \eta_Li$. If the minimum is located at $|\eta| = 1$, only two parameters are necessary.

The Hamiltonian describing a motion in $\eta$ has the following form:

$$H = -\frac{\hbar^2}{2B_\eta} \frac{d^2}{dx^2} + U(x, I),$$

(5)
where $B_\eta$ is a constant effective mass parameter. The method of calculation of the mass parameters for the DNS is given in [25]. Calculations show that $B_\eta$ is a smooth function of the mass number. Since we study nuclei in the same mass region, we take $B_\eta = 20 \times 10^4 m_0$ fm$^2$ for all considered nuclei. Using this value of $B_\eta$ and the connection between mass asymmetry and multipole expansion coordinates of Ref. [16], one can find that the mass parameter for $\beta_3$ vibrations is close to the value $200$ $\hbar^2$/MeV known in literature [17]. Solving the eigenvalue problem of the Hamiltonian (5), we obtain the spectrum of $\eta$-vibrations and the parity splitting as a function of $I$.

The eigenfunctions of the Hamiltonian (5) have a well defined parity with respect to $x \rightarrow -x$ reflection. The change of the sign of $x$ is equivalent to the change of the sign of $\eta$ and therefore is equivalent to the spatial reflection because, as it is seen from the definition of $\eta$, the change of the sign of $\eta$ is equivalent to the permutation of clusters.

Results of the calculations are shown in Figs. 1–3. They demonstrate a good agreement with the experimental data [26] for all nuclei considered excluding the lightest isotopes of Ra. A satisfactory description of the experimental data, especially of the variation of
the parity splitting at low $I$ and of the value of the critical spin at which the parity splitting disappears with $A$ means that the variation of the potential energy as a function of $\eta$ and $I$ for the isotopes of Ra, Th and U is correctly described by our cluster model. The use of the correct value of the inertia coefficient $B_\eta$ is also important. For the same potential energy with a minimum at $\eta = \eta_\alpha$, we can obtain a maximum of the ground state wave function at about $|\eta| = 1$ for small $B_\eta$ or a concentration of the ground state wave function near $|\eta| = \eta_\alpha$ for very large $B_\eta$.

The calculated ground state wave function has its maximum in the vicinity of $|\eta| = 1$ even when the potential energy has a minimum at $\eta = \eta_\alpha$ because this minimum is rather shallow (it does not exceed 0.8 MeV), and the inertia coefficient $B_\eta$ used in the calculations is not large (see Fig. 4). Thus, the ground state energy level lies near the top of the barrier and the estimated weight of the $\alpha$-cluster configuration is about $2 \times 10^{-2}$ for $^{226}$Ra, that is close to the calculated spectroscopic factor [27]. This means that our model is in agreement with the known $\alpha$-decay widths for the nuclei considered.

Using the wave functions obtained, we calculated the multipole moments $Q_1$, $Q_2$, $Q_3$ and $Q_4$. The obtained values are in good agreement with the known experimental data for $Q_j^{\text{exp}}$ [2]. For example, for $^{226}$Ra we find $Q_1 = 0.10$ e fm ($Q_1^{\text{exp}} = 0.1$ e fm) $Q_2 = 740$ e fm$^2$ ($Q_2^{\text{exp}} = 750$ e fm$^2$), $Q_3 = 3200$ e fm$^3$ ($Q_3^{\text{exp}} = 3100$ e fm$^3$) and $Q_4 = 19,000$ e fm$^4$. These first results allow us to hope for a good description of transitions probabilities $B(E_\lambda)$ and multipole moments $Q_j$ for different isotopes of Ra, Th and U in a forthcoming publication.

In conclusion, we suggested a cluster interpretation (oscillations in the mass asymmetry coordinate) of the parity splitting in different Ra, Th and U isotopes. The existing experimental data on the spin dependence of parity splitting were quite well described. The characteristics of the Hamiltonian used were determined by investigations of completely different phenomena, namely, heavy ion reactions at low energies.

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