Cluster approach to the structure of heavy nuclei

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Abstract. We developed a cluster model which allows to take into account both shape deformation parameters and cluster degrees of freedom. The important ingredient of the model is the dinuclear system concept in which the wave function of the nucleus is treated as a superposition of a mononucleus and two-cluster configurations. The model is applied to describe the multiple negative-parity bands in the deformed actinides.

1. Introduction

In the even–even isotopes of actinides and also in the heavy Ba and Ce isotopes the low-lying negative parity states are observed in the rotational or quasirotational bands. While the formation of the positive-parity bands is connected in general to the quadrupole collective motion, the lowering of the states with negative-parity is a signature of the reflection asymmetric collective mode.

There are several approaches to treat the collective motion related to the reflection asymmetric degrees of freedom (see [1] and references therein). In present work, we use the ideas of the model developed in [2] that the collective oscillations of the nucleus in the mass asymmetry degrees of freedom lead to the formation with some probability of the cluster-type configurations. The contribution of the asymmetric cluster configurations to the intrinsic nuclear wave function simultaneously creates deformations with even and odd–multipolarities. The idea that the motion in mass asymmetry is responsible for the reflection–asymmetric deformations of the medium mass and heavy nuclei is based on the fact that these nuclei are good alpha-emitters.

In [2], only the lowest negative parity bands ($K^\pi=0^–$) have been considered. However, there are experimental evidences of the negative-parity collective states characterized by non zero values of $K$ (see, for example, [3]). Moreover, the recent investigations [4] have indicated that the reflection-asymmetric degrees of freedom can also contribute significantly to the structure of positive parity rotational band built upon excited $0^+_2$ state which are observed in the excitation spectra of many actinides.

To treat these collective excitations in the framework of our cluster approach, we modify the cluster model [2] to take into account the intrinsic excitations of clusters produced by the motion in mass-asymmetry degrees of freedom. In [5], we applied the modified model to treat the properties of $^{220}$Th. This is a peculiar case of the nucleus characterized by the strong
reflection-asymmetric deformation and relatively small quadrupole deformation. The aim of this work is to treat the situation when the nucleus has both strong quadrupole and strong reflection-asymmetric deformations. The model is applied to the description of the multiple reflection-asymmetric bands in heavy isotopes of actinides.

2. Model

Instead of parametrizing nuclear shapes in terms of multipole deformation parameters, we use the degrees of freedom related to the dinuclear system (DNS). Under the expression of dinuclear system we understand the system of two touching fragments \((A_1, Z_1)\) and \((A_2, Z_2)\) with \(A_1 + A_2 = A\) and \(Z_1 + Z_2 = Z\) kept together by the molecular-type nucleus-nucleus potential. The special case of the DNS in which one fragment has zero mass is denoted as a mononucleus. Each dinuclear system configuration can be characterized by the mass-asymmetry \(\xi = 2A_2/A\), charge-asymmetry \(\xi_Z = 2Z_2/Z\) and the vector of the relative distance \(\mathbf{R} = (R, \theta, \phi)\).

The main idea of the DNS model is that the intrinsic nuclear wave function can be presented as a superposition of the mononucleus and different dinuclear configurations. The mononucleus is taken to be quadrupole-deformed; thus, in the DNS model, the reflection-asymmetric deformation of the nucleus related solely to the non zero weight of the asymmetric dinuclear systems.

Applying the model to the description of the low-lying excitations in actinides, we presume that the main source of the reflection asymmetric deformation is the contribution of the DNS with an alpha-particle as a light cluster. This idea is related to the experimental observation that the actinides are good \(\alpha\)-emitters. Thus, there is a significant probability to form an \(\alpha\)-cluster in the surface region of the nucleus. Due to the stable closed-shell structure of the nucleus, it is reasonable to presume that the ground-state and low-lying excited states of actinides can have a significant contribution of \(\alpha + (A - 4, Z - 2)\) cluster structures (\(\alpha\)-cluster DNS) without appreciable internal excitations of the heavy fragment.

The degrees of freedom chosen to characterize a system with quadrupole deformed heavy cluster and spherical light cluster are related to the transfer of nucleons between the fragments, to the rotation of the heavy fragment, and to the relative motion of fragments. The charge asymmetry \(\xi_Z\) is not considered as an independent collective variable, and fixed to minimize the symmetry energy of the DNS for each value of \(\xi\).

The Hamiltonian of the model has the form

\[
\hat{H}_0 = -\frac{\hbar^2}{2B_\xi} \frac{1}{\xi^{3/2}} \frac{\partial}{\partial \xi} \xi^{3/2} \frac{\partial}{\partial \xi} + \frac{\hbar^2}{2\Im_h(\xi)} \hat{l}_k^2 + \frac{\hbar^2}{2\mu(\xi)R_m^2} \hat{r}_0^2 + \frac{\hbar \omega_R(\xi)}{2} + U(\xi, R_m, \beta_0, \epsilon). \tag{1}
\]

Here, we assumed that the value of the internuclear distance \(R = R_m(\xi, \beta_0, \epsilon)\) is set to be equal to the position of the minimum of the potential in \(R\) for given values of \(\xi\), relative orientation of the fragments defined by angle \(\epsilon\) and the deformation \(\beta_0\) of the heavy cluster. The calculations of the potential energy \([6]\) show that the minimum corresponds to the touching configuration of the clusters. \(\hbar \omega_R(\xi)/2\) is the energy of the zero-order vibrations in \(R\) around the equilibrium value \(R_m\). We treat mass-asymmetry \(\xi\) as a continuous variable.

In eq. (1), \(\mu \approx m_0 A_{\xi}/2\) is the reduced mass of the DNS (\(\xi \ll 1\)), \(m_0\) is the nucleon mass, and \(\Im_h(\xi)\) is the moment of inertia of the heavy fragment. The \(\hat{l}_k^2\) are the operators of the square of the angular momentum of the rotation of the heavy fragment \((i = h)\) and of the relative rotation of the two clusters \((i = 0)\):

\[
\hat{l}_k^2 = -\frac{1}{\sin \theta_i} \frac{\partial}{\partial \theta_i} \sin \theta_i \frac{\partial}{\partial \theta_i} - \frac{1}{\sin^2 \theta_i} \frac{\partial^2}{\partial \phi_i^2}. \tag{1}
\]

The angles \(\hat{\Omega}_i = (\theta_i, \phi_i)\) describe the orientation of the symmetry axis of the heavy fragment \((i = h)\) and of the vector \(\mathbf{R}\) \((i = 0)\) with respect to the laboratory frame. The angle of relative orientation \(\epsilon\) can be related to \(\Omega_0\) and \(\Omega_h\) by the expression \(\sin^2 \epsilon = (2/3)(1 - \sqrt{3}\left[Y_2(\Omega_h) \times Y_2(\Omega_0)\right]_{(00)})\).
The calculation of the mass parameter $B_\xi$ is given in [7]. In this work, we take $B_\xi = (10 - 20) \times 10^5 m_0$ fm$^2$. One should note that this value is larger than those used in our previous calculations [2] because of the fact that additional degrees of freedom are considered and renormalize of the mass tensor.

The potential energy $U(\xi, R_m, \beta_0, \epsilon)$ is determined as

$$U(\xi, R_m, \beta_0, \epsilon) = B_1(\xi) + B_2(\xi) + V(\xi, R_m, \beta_0, \epsilon),$$

where the quantities $B_1, B_2$ are the binding energies of the clusters forming the DNS. The experimental ground–state masses [8], if available, are used in the calculations. If not, the predictions of [9] are used. Shell effects and pairing correlations are included in the binding energies. The nucleus-nucleus potential $V(R = R_m, \xi, \beta_0, \epsilon)$ is calculated using the procedure described in [6].

The potential energy as a function of relative orientation of the fragments has a minimum which corresponds to the pole-to-pole orientation ($\epsilon = 0$). We approximate the $\epsilon$-dependence of the potential energy by the second order expansion in the Legendre polynomials as

$$U(\xi, R_m, \beta_0, \epsilon) = U_0(\xi, R_m, \beta_0) + C_0(R_m, \beta_0)\xi \sin^2 \epsilon$$

$$= (U_0 + (2/3)C_0\xi) - (2/3)\sqrt{C_0} [Y_2(\Omega_h) \times Y_2(\Omega_0)]_{(00)},$$

where $U_0(\xi, R_m, \beta_0) = U(\xi, R_m, \beta_0, \epsilon = 0)$. Since $\xi \ll 1$, we expand the interaction term in (3) leaving only term linear in $\xi$, that is $C_0(R_m, \xi, \beta_0) \approx C_0(R_m, \beta_0)\xi$. The value of $C_0(R_m, \beta_0)$ is fixed by fitting $\epsilon$-dependence of the potential energy $U$ calculated with eq. (2). The potential energy of the mononucleus configuration ($\xi = 0$) which can not be calculated with eq. (2) is fitted to reproduce the correct value of the nuclear binding energy as the lowest eigenstate of the Hamiltonian (1).

The Hamiltonian (1) is diagonalized on the set of basis functions

$$\Phi_{LM, n}^{l_1 l_2} = F_n(\xi) [Y_{l_1}(\Omega_h) \times Y_{l_2}(\Omega_R)]_{(LM)},$$

where $n=0,1,2,...$, $l_1=0,2,4,...$, $l_2=0,1,2...$ The angular part of the wave function (4) is given by the bipolar spherical harmonics, which provide the proper transformation with respect to the rotation and space inversion. Since we have assumed that the heavy fragment is the axially–symmetric quadrupole rotator the quantum number $l_1$ can take only even values. The parity of the state is then determined as $\pi = (-1)^{l_2}$.

3. Calculated results

The calculations of the energy spectra are presented in fig. 1 together with available experimental data for $^{230}$Th, $^{232}$U, $^{238}$U, and $^{240}$Pu nuclei. The experimental energies, spins, and parities are taken from [10]. One can see that the structures of the spectra are very similar for all considered nuclei. To elucidate the peculiarities of the calculated spectra, one can examine which basis function from the set (4) mostly contributes to the wave functions of the states of different rotational bands.

For the ground-state rotational band, the angular part of the wave-function of the state with angular momentum $L$ is close to the function $[Y_{l_1=0}(\Omega_h) \times Y_{l_2=0}(\Omega_0)]_{(L,M)}$. Since $\pi = (-1)^{l_2}$, the ground-state band contains only the states of positive parity with even angular momentum $L$. The wave functions of the lowest negative parity states have the dominant component $[Y_{l_1=L}(\Omega_h) \times Y_{l_2=1}(\Omega_0)]_{(L+1,M)}$. They form a rotational band which contain the states of odd angular momentum and negative parity. This band can be interpreted as $K^\pi = -^-$ band. One should note, however, that each eigenfunction of Hamiltonian (1) is a superposition of
the states with different $K$ values, thus $K$ can be considered as a quantum number only approximately. The next lowest band of negative parity is formed from the states with main contribution of $[Y_{l_1=1}(\Omega_h) \times Y_{l_2=1}(\Omega_0)]_{(L-1,M)}$ component for odd angular momentum and $[Y_{l_1=1}(\Omega_h) \times Y_{l_2=1}(\Omega_0)]_{(L,M)}$ component for even angular momentum. This band can be approximately interpreted as $K^\pi = 1^-$. In this case the angular momentum carried by the relative rotation is directed oppositely with the total angular momentum, thus, shifting up the energy of this rotational band with respect to the $0^-\pi$ band. The first excited $0^+\pi$ state is obtained as a lowest excitation in the mass-asymmetry coordinate.

As seen in fig. 1, the agreement between the calculated excitation spectra and corresponding experimental rotational bands are rather good for all presented nuclei. One can notice, however, that some of the bands, measured experimentally, namely, $K^\pi=0^+,2^+$, and $2^-\pi$ rotational bands, are absent in the calculated spectra. The reason for this is that in the present version of the model we have considered the heavy fragment with stable axially-symmetric quadrupole deformation. Thus, we may expect, that if we add into consideration the $\beta-$ and $\gamma-$ vibrations of the heavy fragment, the calculated spectra of actinides will contain additional $0^+$ and $2^+$ rotational bands, which are build on the $\beta$ and $\gamma-$vibrational excitations, respectively. We can also expect, the appearance of additional low-lying $0^-$ and $2^-\pi$ bands, as a negative parity doublets to the $0^-\pi$ and $2^-\pi$-vibrational bands. Note that the alternative way to explain the low-lying $2^-\pi$ bands in actinides is based on the concept of tetrahedral deformation [11, 12].

The interesting quantity is the parity splitting defined as the energy shift between the states of $0^-\pi$ and $0^+\pi$ rotational bands. The dependences of the experimental and calculated values of a parity splitting in the ground state and the first negative parity bands (they are treated as a unified alternating parity band) on angular momentum are shown in fig. 2. The parity splitting is defined by the expression [3]:

$$S(I^-) = E(I^-) - \frac{(I + 1)E^{+}_{(I-1)} + IE^{+}_{(I+1)}}{2I + 1},$$

which provides zero value of parity splitting for the rotational band of nucleus with rigid octupole deformation. Having maximum value in the beginning of the band, the parity splitting decreases with increasing angular momentum. In our model the value of parity splitting is determined by
the relative weights of the cluster components and the mononucleus in the wave function. Due to the larger moment of inertia the weight of \(\alpha\)-particle DNS increases with angular momentum that decreases the parity splitting.

4. Conclusion
We have suggested a cluster interpretation of the properties of the multiple negative parity bands in deformed even–even actinides. The collective motion related to the cluster degree of freedom leads to the admixture of the very asymmetric cluster configurations to the intrinsic nucleus wave function. To take into account the reflection asymmetric modes with nonzero values of \(K\), the rotational excitations of the heavy cluster are taken into account. The resulting energy spectrum consists of the ground state band, the excited \(0^+\) band and several negative parity rotational bands which can be approximately interpreted as \(K^{\pi} = 0^-\) and \(K^{\pi} = 1^-\) bands. The angular momentum dependence of the parity splitting is described. The results of calculations are in good agreement with the experimental data.

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