Rotation Modes in the Dinuclear Model

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Abstract. The dinuclear system model can be applied to nuclear structure. Here we study deformed clusters which rotate with respect to the internuclear distance and exchange nucleons. The model is used to explain the band structure of nuclear spectra, e. g. the parity splitting observed in 238 U.

1 Introduction

A nuclear molecule or a dinuclear system (DNS) consists of a configuration of two touching nuclei (clusters) which keep their individuality. Such a system has two main degrees of freedom which govern its dynamics: (i) the relative motion between the nuclei describing the formation and decay of the dinuclear system and (ii) the transfer of nucleons between the nuclei. The latter process changes the mass and charge asymmetries which are defined by the coordinates

$$\eta = \frac{A_1 - A_2}{A_1 + A_2}$$
 and $\eta_Z = \frac{Z_1 - Z_2}{Z_1 + Z_2}$. (1)

These coordinates can be assumed as continuous or discrete quantities. For $\eta = \eta_Z = 0$ we have a symmetric clusterization with two equal nuclei, and if η approaches the values ± 1 or if A_1 or A_2 is equal to zero, a fused system has been formed.

The DNS concept was suggested by V. V. Volkov [1, 2] to explain fusion reactions. In the meantime the DNS model has been applied to a large variety of nuclear phenomena where cluster features play a dominant role. For nuclear structure it has been used to describe the parity splitting [3, 4], normal- and superdeformed bands [5,6] and the appearance of hyperdeformed states as nuclear molecular structures in heavy ion collisions [7]. As an example for parity splitting, we list in Table 1 the levels of the positive parity ground state and shifted negative parity rotational bands of N = 152 isotones, which are calculated with the DNS model and compared with available experimental data.

The DNS model found numerous applications in the prediction of the fusion dynamics of heavy ions forming superheavy nuclei [8,9] and in describing the accompanied quasifission process [10]. Also the binary and ternary fission processes of heavy nuclei have been treated with the DNS model [11].

Ι	²⁴⁸ Cm	Í	250 Cf	I	252 Fm		254 No	
	E	$E_{\rm exp}$	E	$E_{\rm exp}$	E	$E_{\rm exp}$	E	$E_{\rm exp}$
0^+	0	0	0	0	0	0	0	0
1-	865	1049	823		811		773	
2^{+}	43	43	43	43	47	47	44	44
3-	930	1094	888		881		838	
4^+	143	144	143	142	155		146	145
5^{-}	1046	1172	1003		1003		954	
6^+	298	298	297	296	322		304	304
7^{-}	1211		1167		1177		1119	
8+	504	505	503	500	544		516	518
9-	1423		1375		1398		1330	
10^{+}	760	761	757		818		780	786
11^{-}	1677	1680	1625		1661		1583	
12^{+}	1061	1061	1056		1138		1091	1104
13-	1970	1938	1912		1963		1876	
14^{+}	1404	1403	1394		1500		1445	1470
15^{-}	2299	2238	2233		2297		2203	
16^{+}	1784	1780	1767		1899		1838	1884
17^{-}	2658	2574	2583		2659		2560	
18^{+}	2197	2188	2175		2330		2267	2340
19-	3045	2944	2957		3044		2942	
20^{+}	2641	2622	2609		2787		2725	2839

Table 1. Calculated (*E*) and experimental (E_{exp}) energies (in keV) of the levels of the ground state and first negative parity rotational bands ($K^p = 0^+$) in N = 152 isotones. Experimental data are taken from http://www.nndc.bnl.gov/nndc/ensdf/.

2 Rotation Modes in the Dinuclear Model

The clusters of the dinuclear system model are assumed to be deformed and to rotate. In this case we have to discriminate three different coordinate systems: (i) the space-fixed system with its origin at the center of mass, (ii) the molecular system where the z'-axis is defined by the direction of the internuclear distance \mathbf{R} , (iii) body-fixed systems of clusters with axes x_1'', y_1'', z_1'' and x_2'', y_2'', z_2'' which are the principal axes for the tensors of the moments of inertia of clusters 1 and 2, respectively. If we include the mass asymmetry motion and β - and γ -vibrations, we can write the general Hamiltonian as follows:

$$H = \frac{p_R^2}{2\mu_{RR}} + \frac{L^2 - L_{z'}^2}{2\mu_{RR}R^2} + \frac{p_\eta^2}{2B_{\eta\eta}} + \sum_{i=1}^3 \frac{I_i^{(1)2}}{2\Im_i^{(1)}} + \sum_{i=1}^3 \frac{I_i^{(2)2}}{2\Im_i^{(2)}} + T_{vib}(\beta_1, \gamma_1) + T_{vib}(\beta_2, \gamma_2) + \text{kinetic coupling terms} + U(R, \eta, \text{orientation angles}, \beta_1, \gamma_1, \beta_2, \gamma_2).$$
(2)

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Here, L is the angular momentum of the molecular system and $I_{i=1,2,3}^{(1) \text{ or } (2)}$ are the angular momentum components for the rotation of the clusters 1 or 2, respectively, with respect to the axes of the body-fixed systems of the clusters. The angular momentum L of the molecular system is connected with the reduced mass μ_{RR} of the internuclear motion, depending on η and R. The total angular momentum of the system is given as

$$J = L + I^{(1)} + I^{(2)}.$$
 (3)

Further, $B_{\eta\eta}$ is the mass for the mass asymmetry motion. For large mass asymmetries, i. e. $1 - |\eta| \ll 1$, $B_{\eta\eta}$ can be estimated by relating the mass asymmetry coordinate η to the octupole deformation coordinate β_3 . Such a relation between η , R and β_3 was derived in [12]:

$$\beta_3 = -\sqrt{\frac{7}{4\pi}} \frac{\pi}{3} \eta (1 - \eta^2) \frac{R^3}{R_0^3},\tag{4}$$

where R_0 is the spherical equivalent radius of the corresponding compound nucleus. If we take the value of $B_{\beta_3} = 200\hbar^2 \text{ MeV}^{-1}$ known from the literature [13], then we obtain $B_{\eta\eta} \approx (d\beta_3/d\eta)^2 B_{\beta_3} = 9.3 \times 10^4 M \text{ fm}^2$ (*M* is the nucleon mass), compatible with the one used in calculations [4].

The kinetic coupling terms in (2) are manifold. They describe the kinetic coupling between the internuclear, mass asymmetry, β - and γ -vibrational and rotational motions of the clusters and will be not further specified here (see for example [14]). Under the assumption of a small overlap of the nuclei in the DNS, the potential energy U is usually semi-phenomenologically calculated [15]

$$U = B_1 + V_1(\beta_1, \gamma_1) + B_2 + V_2(\beta_2, \gamma_2) - B_{12} + V(R, \eta, \text{orientation angles}, \beta_1, \gamma_1, \beta_2, \gamma_2).$$
(5)

Here, B_i (i = 1, 2) are the experimental mass excesses (negative binding energies) of the clusters and B_{12} of the compound nucleus, and V_i (i = 1, 2) are the potentials for the individual nuclei depending on the quadrupole deformation coordinates. Vis the interaction between the nuclei, $V = V_C + V_N$, consisting of the Coulomb and nuclear potentials. The nuclear part is calculated by a double folding procedure with a Skyrme-type effective density-dependent nucleon-nucleon interaction taken from the theory of finite Fermi systems [16] and with realistic nuclear density distributions for the clusters. Also the deformations of the clusters have to be taken into account.

The rotation energy can be transformed to the molecular coordinate system

$$T_{rot} = \frac{1}{2\mu_{RR}R^2} \left((J_{x'} - I_{x'}^{(1)} - I_{x'}^{(2)})^2 + (J_{y'} - I_{y'}^{(1)} - I_{y'}^{(2)})^2 \right) + \sum_{i=1}^3 \frac{I_i^{(1)2}}{2\Im_i^{(1)}} + \sum_{i=1}^3 \frac{I_i^{(2)2}}{2\Im_i^{(2)}},$$
(6)

where $I_{x',y',z'}^{(1) \text{ or } (2)}$ are the components of the angular momenta $I^{(1)}$ and $I^{(2)}$ of the clusters which are related by an orthogonal transformation, depending on the angles of the body-fixed systems with respect to the molecular system.

$$I_{x'(y',z')}^{(j)} = \sum_{i=1}^{3} R_{x'(y',z'),i}^{(j)} I_{i}^{(j)} \quad \text{with} \quad j = 1 \text{ or } 2.$$
(7)

The terms containing the products of $J_{x',y'}$ and $I_{x',y'}^{(1) \text{ or } (2)}$ in T_{rot} constitute the so called Coriolis interaction which is strongly contributing in molecular systems and can be partly approximated by introducing the total moment of inertia of the system as shown next.

A simplified example for a molecular rotation helps to clarify the problems inherent in the Coriolis interaction. Let us consider the rotation of two bodies around the space-fixed z-axis with polar angles φ_1 and φ_2 with respect to the space-fixed x-axis. These two bodies have moments of inertia $\Im^{(1)}$ and $\Im^{(2)}$, respectively. In the space-fixed coordinate system the rotation energy is

$$T_{rot} = \frac{J_{\varphi_1}^2}{2\Im^{(1)}} + \frac{J_{\varphi_2}^2}{2\Im^{(2)}} \tag{8}$$

with the angular momenta J_{φ_1} and J_{φ_2} . The total angular momentum is given by $J = J_{\varphi_1} + J_{\varphi_2}$. If we denote the direction fixed by the angle φ_1 as molecular axis and transform T_{rot} to the molecular system by $\vartheta = \varphi_1$ and $\varphi = \varphi_2 - \varphi_1$, we obtain

$$T_{rot} = \frac{(J - J_{\varphi})^2}{2\Im^{(1)}} + \frac{J_{\varphi}^2}{2\Im^{(2)}},\tag{9}$$

where $J = J_{\vartheta}$ is the total angular momentum. The first term in T_{rot} contains the important Coriolis coupling connected with the moment of inertia $\mathfrak{S}^{(1)}$. In this simple example the Coriolis coupling term can be transformed away by introducing the new coordinates

$$\vartheta' = \vartheta + \frac{\varphi}{1 + (\Im^{(1)}/\Im^{(2)})} \quad \text{and} \quad \varphi' = \varphi.$$
 (10)

We obtain

$$T_{rot} = \frac{J^2}{2(\mathfrak{S}^{(1)} + \mathfrak{S}^{(2)})} + \frac{1}{2} \left(\frac{1}{\mathfrak{S}^{(1)}} + \frac{1}{\mathfrak{S}^{(2)}} \right) J_{\varphi'}^2.$$
(11)

Now we have reached the result that the term containing the square of the total angular momentum appears with the total moment of inertia $\Im^{(1)} + \Im^{(2)}$ and the second term contains an inverse reduced moment of inertia $\Im^{(1)-1} + \Im^{(2)-1}$. Such a transformation is not possible in three dimensions. However, we can approximate the effects of the Coriolis coupling in (6) with an expression of the form

$$(J^2 - J_{z'}^2)/(2\Im_{tot}),$$
 (12)

where \Im_{tot} is an effective total moment of inertia of the system around an axis perpendicular to the molecular axis.

The moment of inertia \Im_{tot} can be expressed for very asymmetric cluster configurations, e. g. with α and Li as light clusters, as

$$\Im_{tot}(\eta) = c_1 \Big(\Im_1^r + \Im_2^r + M \frac{A_1 A_2}{A} R^2 \Big).$$
(13)

Here, \Im_i^r (i = 1, 2) are the rigid body moments of inertia for the clusters of the DNS, $c_1 = 0.85$ for all up to now considered nuclei. Single particle effects like alignment of the single particle angular momenta in the heavy cluster are neglected. For $|\eta| = 1$, the moment of inertia is not known from the data because the experimental moment of inertia is a mean value between the moments of inertia of the mono-nucleus $(|\eta| = 1)$ and of the cluster configurations arising due to oscillations in η . We assume $\Im_{tot}(|\eta| = 1) = c_2 \Im^r(|\eta| = 1)$ where \Im^r is the rigid body moment of inertia of the mono-nucleus calculated with the deformation parameters and $c_2 = 0.1 - 0.3$ a scaling parameter fixed by the energy of the first 2^+ state.

The Hamiltonian (2) without the mass asymmetry motion and the γ -vibrations was, for example, applied to resonances observed in the scattering of ²⁴Mg on ²⁴Mg [17, 18]. These resonances have widths of about 200 keV and angular momenta of 36-42 \hbar at incident energies $E_{c.m.} = 42 - 56$ MeV [19]. They can be explained by molecular states in pole-to-pole-like configurations of the ²⁴Mg nuclei.

3 Application to Nuclear Structure of ²³⁸U

In this Section we apply the Hamiltonian of the dinuclear model to the case of large mass asymmetries and describe low-lying bands in ²³⁸U. We assume that the clusterization can vary and consists of a heavy cluster with an axially symmetric quadrupole deformation β and of spherical light clusters, e.g. an alpha-particle. The internuclear distance coordinate $R = R_m$ is chosen as fixed at the touching configuration which is determined by the minimum of the potential of the DNS in the internuclear coordinate R. Then the degrees of freedom are: (i) rotation of the heavy cluster about an axis perpendicular to its symmetry axis, this axis is fixed by the angles ϑ_1 and φ_1 in the space-fixed system, (ii) rotation of the molecular system, defined by the direction of \mathbf{R} with the angles ϑ_2 and φ_2 in the space-fixed system, (iii) mass asymmetry motion described by a new mass asymmetry coordinate with positive values only:

$$\xi = 2A_2/A = 1 - \eta. \tag{14}$$

The total Hamiltonian is assumed as

$$H = \frac{J_1^2}{2\Im_h} + \frac{J_2^2}{2\mu_{RR}(\xi)R_m^2} - \frac{\hbar^2}{2B}\frac{1}{\xi}\frac{\partial}{\partial\xi}\xi\frac{\partial}{\partial\xi} + U(\xi,\varepsilon),$$
(15)

where

$$J_i^2 = -\hbar^2 \left(\frac{1}{\sin \vartheta_i} \frac{\partial}{\partial \vartheta_i} \sin \vartheta_i \frac{\partial}{\partial \vartheta_i} + \frac{1}{\sin^2 \vartheta_i} \frac{\partial^2}{\partial \varphi_i^2} \right) \quad \text{with} \quad i = 1, 2.$$
(16)

Here, \Im_h is the moment of inertia of the heavy cluster fixed from a comparison with the energy of the lowest experimental and calculated 2^+ state. The spherical light cluster has $\Im_{\ell} = 0$. Further, J_1^2 and J_2^2 are the squares of the angular momentum operators of the rotation of the heavy cluster and of the internuclear distance \mathbf{R} (rotation in the relative motion of light cluster), respectively, described in the spacefixed coordinate system. The potential energy is a sum of two terms: a power series expansion in the mass asymmetry coordinate ξ and an interaction energy depending on the difference angle ε between (ϑ_1, φ_1) and (ϑ_2, φ_2) which is the angle between the internuclear distance \mathbf{R} and the symmetry axis of the heavy fragment:

$$U = \sum_{n=0}^{3} a_n \xi^{2n} + \frac{C_0}{2} \xi \sin^2(\varepsilon)$$
 (17)

with

$$\sin^2(\varepsilon) = \frac{2}{3} \left(1 - \frac{4\pi}{\sqrt{5}} [Y_2(\vartheta_1, \varphi_1) \otimes Y_2(\vartheta_2, \varphi_2)]_{(0,0)} \right). \tag{18}$$

If the parameter C_0 is small, the two rotation degrees of freedom are approximately independent. For large C_0 , the symmetry axis of the heavy deformed cluster is essentially directed towards the light cluster and bending oscillations of the heavy cluster around the molecular axis occur. Spectra resulting from smaller and larger C_0 values will be discussed below.

The Hamiltonian (15) can be diagonalized. Then the wave function results in the form

$$\Psi_{JM} = \sum_{\kappa, J_1, J_2} c_{\kappa, J_1, J_2, J} \phi_{\kappa}(\xi) [Y_{J_1}(\vartheta_1, \varphi_1) \otimes Y_{J_2}(\vartheta_2, \varphi_2)]_{(J,M)},$$
(19)

where the functions $\phi_{\kappa}(\xi)$ form a basis set for the bound mass asymmetry motion. Since the heavy cluster can have only even nuclear spin values, the parity of Ψ_{JM} is determined by the wave function of the molecular motion consisting of a rotation in the relative motion of the light cluster: $P = (-1)^{J_2}$.

Let us consider the level spectrum for $C_0 = 0$ with a fixed value of $\xi = \xi_0$. In this case the ground state band with states of positive parity originates from the rotation of the heavy cluster only with $J_1 = 0, 2, 4, ...$, and the rotation of the molecular axis is zero ($J_2 = 0$). We note that the relation of moments of inertia is $\Im_h(\xi) > \mu_{RR}(\xi)R_m^2$. Therefore, the first excited band with states of negative parity is built on a rotation of the molecular axis with $J_2 = 1$. These states are degenerated with spins $1^-, (1^-, 2^-, 3^-), (3^-, 4^-, 5^-), ...$ If C_0 starts to increase, the considered negative parity states lose their property of degeneracy and are shifted. This effect is recognizable in Figure 1 where we compare the experimental energy



Figure 1. The experimental and calculated level spectra of 238 U. In the diagonalization of H (Eq. (15)) a smaller parameter C_0 is used. The mass asymmetry motion is included. Experimental data are taken from http://www.nndc.bnl.gov/nndc/ensdf/.

spectrum of ²³⁸U with the spectrum calculated within this model. Here, the parameter C_0 has a smaller value. The first excited 0^+ state results from the first excited state in the mass asymmetry motion on which the lower spectrum is approximately repeated again (ground state band and 1^- band starting at 1386 keV).

For larger C_0 values, the first negative parity band is shifted downwards and we obtain bending oscillations of the heavy cluster with a small angle ε . The rotational part of the Hamiltonian can be transformed for fixed mass asymmetry ($C = C_0 \xi_0$) as follows:

$$H = H_{rot} + H_{bend} + V_{int},\tag{20}$$

where

$$H_{rot} = \frac{1}{2\mu_{RR}R_m^2} \left(J^2 - 2J_{z'}^2 \right),$$
(21)

$$H_{bend} = -\frac{\hbar^2}{2\Im_b} \frac{1}{\varepsilon} \frac{\partial}{\partial \varepsilon} \varepsilon \frac{\partial}{\partial \varepsilon} + \frac{1}{2\Im_b \varepsilon^2} J_{z'}^2 + \frac{C}{2} \varepsilon^2, \qquad (22)$$

$$V_{int} = -\frac{1}{2\mu_{RR}R_m^2} \left(J_{x'}I_{x'}^{(1)} + I_{x'}^{(1)}J_{x'} + J_{y'}I_{y'}^{(1)} + I_{y'}^{(1)}J_{y'} \right).$$
(23)

The moment of inertia of the bending motion is

$$\Im_b = \Im_h \mu_{RR} R_m^2 / (\Im_h + \mu_{RR} R_m^2).$$
(24)



Figure 2. Result of the diagonalization of H (Eq. (15)) without the mass asymmetry dynamics and a larger parameter C_0 for an alpha-particle clusterization of 238 U (234 Th + α).

Approximate eigenenergies can be written as

$$E_{J,M,K,n} = \frac{\hbar^2}{2(\Im_h + \mu_{RR}R_m^2)} (J(J+1) - K^2) + \hbar\omega_b(2n + |K| + 1)$$
(25)

with the oscillator energy of the bending mode

$$\hbar\omega_b = \hbar\sqrt{C/\Im_b} \quad . \tag{26}$$

In order to prove (25), we calculated the energy spectrum by diagonalizing the Hamiltonian (15) disregarding the mass asymmetry motion by assuming an alphaclusterization of ²³⁸U as example. The resulting spectrum shown in Figure 2 is well approximated by (25). The ground state band is an unperturbed alternating parity band as expected in this limit because we have a stable reflection-asymmetric shape. This band does not describe the experimental ground state band of ²³⁸U which contains only states with even spin and positive parity. The next bands have K = 1 and n = 1.

The mass asymmetry coordinate used in this Section assumes positive values, and the light cluster is transferred to the other side of the heavy cluster by rotating it by an angle $\varepsilon = \pi(-\pi)$. This makes it possible to study the dynamics of axially asymmetric dinuclear shapes in greater detail. Depending on the stiffness parameter C_0 , the system has small angular vibrations of the clusters around their equilibrium position for larger values of C_0 and a rotation of the light cluster around the heavy one over a potential barrier at $\varepsilon = \pi/2$ for smaller values of C_0 . The latter case gives a good description of the spectrum of ²³⁸U.

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