Oblate-prolate shape coexistence at finite angular momentum

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We investigate shape coexistence in a rotating nucleus. We concentrate on the interesting case of $^{72}$Kr which exhibits an interesting interplay between prolate and oblate states as a function of angular momentum. The calculation uses the local harmonic version of the method of self-consistent adiabatic large-amplitude collective motion. We find that the collective behaviour of the system changes with angular momentum and we focus on the role of non-axial shapes.

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Only a small number of quantum mechanical many-body systems can be solved exactly through analytical or numerical means. Many approximate schemes exist to find reasonable answers, but these may not always be easy to interpret in physical terms. Another slant on this problem is to try and describe some of the dynamics of such systems in terms of a limited set of degrees of freedom. These should of course be chosen through some method appropriate for the problem at hand. Many approaches are available, in areas ranging from field theories to atomic physics (see, e.g., the reviews in Ref. [1]). These are typically based on the concept of “relevant degrees of freedom”, or on the introduction of collective motion and collective paths – which are two ways to express rather similar principles! Depending on the energy scales involved and the physical situation being described, the remaining degrees of freedom are either frozen out, or treated as a heat-bath for the motion of the relevant degrees of freedom.

The most common description of nuclear collective dynamics is influenced by the success of the liquid drop model [2]. The description is based on the competition between quadrupole shape fluctuations of the nucleus, typically modelled microscopically by a long-range quadrupole-quadrupole force, and a BCS-like pair condensate, modelled by a short-range pairing force. The model of the nucleus does not have to be this naive, but even with better models, it is often assumed that the low-energy dynamics is well described by quadrupole shape fluctuations. We would like to question this assumption, which leads to a search for the best choice of collective coordinates (the standard terminology for the relevant degrees of freedom in this field). There are quite a few partial answers, see the review [3] for a discussion of some of these. The goal is to find a method that determines a collective path self-consistently, based only on knowledge of the Hamiltonian governing the system.

Clearly, in nuclear physics one does not know the Hamiltonian. However, for the collective properties of medium mass to heavy nuclei, models that contain the two key parts of the nuclear force, a short-range pairing force, and a long range multipole-multipole force (usually approximated by a quadrupole-quadrupole one) are known to be able to capture the essential part of the physics, see e.g. the textbook Ref. [4].

With modern experimental techniques, we can create nuclei at considerable angular momentum, and study the behaviour as a function of angular momentum, which provides us with an additional parameter we are almost free to choose. The resulting experimental data are often analysed in terms of simple collective models, usually expressed in terms of quadrupole shapes. The physics of collective motion is then often described in terms of shape transitions and shape coexistence, the mixing between various shapes. One important example is the recent large interest in shape coexistence at low angular momentum in nuclei in the $A = 70$ and $N \approx Z$ mass-region [5, 6, 7, 8, 9]. In this region one finds a large diversity of shapes, and rapid changes in shape with particle number and angular momentum. This large variety is caused by shell gaps corresponding to spherical $(N, Z = 38)$, prolate $(N, Z = 34, 38, 40)$ and oblate $(N, Z = 34, 36)$ shapes that exist in this mass-region. The detailed understanding of how states with different shapes mix is, among others, important for the astrophysical nucleosynthesis process that passes through these proton-rich nuclei.

The quality of the recent experimental data, fuelled by advances within the field of $\gamma$-ray spectroscopy, has led to theoretical effort focused on this mass-region. The nucleus $^{72}$Kr, the subject of this letter, shows oblate-prolate shape coexistence and/or shape transitions, the nature of which seems to depend strongly on angular momentum. There are other calculations for this nucleus: Ref. [8] have used the constrained mean-field method to study the potential energy surface. The approach used in Ref. [9] goes beyond the mean field approximation but does not answer the question which degrees of freedom are important for the collective path. Oblate-prolate shape coexistence has also recently been studied in other mass regions, see e.g. Ref. [10].

Our formalism, as set out in detail in Ref. [11], is based on time-dependent mean field theory, and the fact that a classical dynamics can be associated with it. The issue of selecting collective coordinates, and determining their coupling to other degrees of freedom, thus becomes...
an exercise in classical mechanics. If we assume slow motion the mean-field energy, which is also the classical Hamiltonian, can be expanded to second order. This corresponds to a parametrisation of the one-body density matrix in terms of a set of canonical coordinates, $\xi^\alpha$, and conjugate momenta, $p_\alpha$. The potential $V(\xi)$ and the mass matrix $B^{\alpha\beta}(\xi)$ are the coefficients of the expansion of the classical Hamiltonian in powers of the momenta $\pi$ at zeroth and second order, respectively. Within this adiabatic Hamiltonian we search for collective (and non-collective) coordinates $q^\mu$ and conjugate momenta $p_\mu$. These are assumed to be obtained by an invertible point transformation of the original coordinates $\xi^\alpha$ and momenta $p_\alpha$, preserving the quadratic truncation of the Hamiltonian dependence of the Hamiltonian, by

$$q^\mu = f^\mu(\xi), \quad p_\mu = g^\mu_\alpha p_\alpha \quad (\mu, \alpha = 1, \ldots, n) \quad (1)$$

where we use a standard notation for the derivatives. The adiabatic Hamiltonian is then transformed into

$$\tilde{H}(q, p) = \tilde{V}(q) + \frac{1}{2} B^{\mu\nu} p_\mu p_\nu + O(p^4) \quad (2)$$

in the new coordinates. The new coordinates $q^\mu$ are now to be divided into three categories: the collective coordinate, the zero-mode coordinates, which describe motions that do not change the energies and finally the remaining non-collective coordinates.

In the local harmonic approximation (LHA) the collective coordinate is determined by means of the solution to a set of self-consistent equations. These are the force equations and the local RPA equation

$$\tilde{H}_{\alpha} = \Lambda f_{\alpha} + \omega J_{x,\alpha} + \sum_{\tau=n,p} \mu_\tau N_{\tau,\alpha}, \quad (3)$$

$$\tilde{V}_{\alpha\beta} B^{\gamma\beta} f_{\gamma} = (\hbar\Omega)^2 f_{\alpha}. \quad (4)$$

The parameters $\omega$ and $\mu$ are Lagrange multipliers that implement the condition of fixed angular momentum along the $x$ axis, and fixed particle number, respectively. In nuclear physics these are usually called generalised cranking parameters. The parameter $\Lambda$ is an additional Lagrange multiplier for the collective mode, forcing the system to stabilise at a point away from equilibrium. The covariant derivative $V_{\alpha\beta}$ is defined in the usual way $^{12}$. The collective path is found by solving Eqs. $^{3}$ and $^{4}$ self-consistently, i.e., we look for a path consisting of a series of points where the lowest non-spurious eigenvector of the local RPA equations also fulfills the force condition. In the minimum of the potential the spurious solutions decouples from the other collective and non-collective solutions. In this paper we have chosen to ignore the effects of the spurious admixtures to the RPA wave-functions, but test calculations has showed these to be small. To limit the computational effort we use the method presented in Ref. $^{11}$ $^{12}$ to reduce the size of the RPA matrix. There it was shown that the RPA equation can be solved with good accuracy by assuming that the RPA eigenvectors can be described as a linear combination of a small number of state-dependent one-body operators. The same basis set turned out to work well also at finite angular momentum.

We apply the LHA to the constrained pairing+quadrupole Hamiltonian as described in $^{12}$ with a constraint on particle numbers and angular momentum

$$H' = h_0 - \sum_{\tau} G_{\tau} P_{\tau}^4 P_{\tau} - \frac{K}{2} \sum_{M=-2}^{2} Q_{M}^{4} Q_{M} - \omega J_{x} - \sum_{\tau} \mu_\tau N_{\tau}, \quad (5)$$

where $h_0$ is the spherical Nilsson Hamiltonian $^{14}$. $Q_{M}$ and $P_{\tau}$ are the dimensionless quadrupole and pairing operators $^{13}$. This Hamiltonian is treated in the Hartree-Bogoliubov approximation, within a model space consisting of two major shells. We follow Ref. $^{13}$ and multiply all quadrupole matrix elements with a suppression factor.

We start by examining the non-rotating states in $^{72}$Kr where a prolate-oblate shape coexistence is established experimentally $^{5}$. We find a collective path going from the oblate minimum over a spherical energy maximum into a prolate secondary minimum and continuing towards larger deformation, see Fig. $^0$. This is in contrast to the result recently found for $^{68}$Se $^{4}$ where the non-rotating prolate and oblate minima are connected via non-axial states. At a value of the collective coordinate $Q \approx 7.5$ there is an avoided crossing between the lowest RPA mode, which we are following, and two higher lying modes that are of pairing vibrational character as can be seen in Fig. $^I$. At this point our algorithm is no longer able to find a stable solution. This indicates that more than one collective coordinate should be used, which at the moment is a very difficult calculation. At large oblate deformation we see a collapse in neutron pairing after an avoided crossing between the $\beta$-vibration we are following and a pairing vibration. As explained in detail in

FIG. 1: Large amplitude collective motion in $^{72}$Kr at $I = 0$. $Q$ is the collective coordinate. a) Energy along the collective path. b) The square of the lowest RPA frequencies. c) The deformation $e_2$ and the triaxiality $\gamma$. d) The dimensionless pairing operators $\langle P_\tau \rangle$. 

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 though it captures much of the physics, is not fully quanti-

FIG. 2: Large amplitude collective motion in $^{72}$Kr at $I = 2$.
See Fig.1 for an explanation of the various figures.

At finite angular momentum the collective path will no longer go through the spherical state, since the rotational energy diverges for such a state. Instead the oblate and prolate minima are connected by a path consisting of non-axial states. Due to problems with narrow level crossings we have to start in both the prolate and oblate minima to find the complete collective path. In Fig. 2 we see that if we start in the (almost) oblate minimum and follow the collective path towards larger oblate deformation the situation is very similar to the non-rotating case discussed above: We first see a decrease in the the quadrupole deformation, but after an avoided crossing with a pairing vibration the collective path changes its nature and ends in a neutron pair-field collapse. When we follow the collective path in the other direction, towards smaller oblate deformation the system goes through an avoided crossing with a $\gamma$-vibrational mode. The path then turns into the triaxial plane and the $\epsilon_2$ deformation is almost constant, but with $\gamma$ decreasing quickly from 60° to 0°. At this point the collective path goes through another avoided crossing this time with a $\beta$-vibration. After the crossing the collective path follows an almost prolate shape with increasing deformation. The number of avoided crossing suggests that our description, even though it captures much of the physics, is not fully quanti-

In Fig. 3 at angular momentum $I = 4$ we see a very different character of the collective path. The collective path is limited by the collapse of both the proton and neutron pair-field. The points of zero neutron or proton pairing has an excitation energy of less the 150 keV. When starting the calculation in the prolate minimum we only find the collective path in a limited region due to avoided crossings. This suggests that this part of the collective dynamics is irrelevant. A related calculation at zero gap, which hardly changes the minimum energy, but has different fluctuations, suggests that there is no collective dynamics around the $4^+$ state calculated here, and thus no shape mixing or shape coexistence.

We want to solve the collective Hamiltonian along the collective path. After having made a semi-classical approximation, which leads to a classical Hamiltonian, we need to remember that we are studying a quantum system. The standard technique to deal with this is to treat the classical Hamiltonian as a quantum one, and to calculate the eigenfunctions and energies. Details on how we do this can be found in Ref. [11]. We have solved the collective Hamiltonian for the $I = 0$, 2 and 4 cases in $^{72}$Kr. We also need to calculate the proton and neutron pairing-rotational masses. They becomes zero at the point where $(P) \rightarrow 0$. In Fig. 4 we see that the ground state wave-function is concentrated in the oblate minimum, but that it has a substantial spread along the collective path and is skewed towards the spherical state due to the collapse in the neutron pair-field. The first excited $I = 0$ state has its major component in the prolate minimum with a small component in the oblate minimum. The prolate peak in the wave-function for the first excited state is broader and more symmetric than for the ground state. The third $I = 0$ state is approximate spherical but has substantial oblate as well as prolate components. The prolate state lies at a very low excitation energy of only 0.37 MeV, while the spherical state is somewhat higher in energy. For $I = 2$ the situation is similar to the case $I = 0$. However, the mixing of the prolate and oblate states is substantially stronger. The long tail of the oblate peak stretches along the collective path into the prolate minimum, and that there is a secondary oblate peak in the prolate state. Due to the wide peaks of the collective wave function the expectation value of deformation in the collective states are substantially different from those of the minimum potential energy states, as can be seen in Table II. Note that even though the mean-field results show an almost axially symmetric solution at $I = 2$ ($\gamma < 1^\circ$) the collective state shows a substantial $\gamma$-deformation. For the $I = 4$ state the situation is different. We can use the pairing collective paths, but these are limited by the pairing collapse. Therefore we do not see any low lying excited states and we see no
FIG. 4: The wave function for the large amplitude collective motion in $^{72}$Kr at $I = 0$ and 2 as a function of the collective coordinate $Q$. The thick solid line is the potential energy. The wave functions have their scale on the right side.

TABLE I: The deformation and excitation energy (in MeV) for the collective states.

| $I_\pi$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|--------|---|---|---|---|---|---|---|
| $\varepsilon_2$ | 0.28 | 0.37 | 0.30 | 0.40 | 0.36 | 0.36 | 0.45 |
| $\gamma$ | 60.0 | 0.0 | 0.0 | 42.4 | 9.8 | 19.9 | 59.3 |
| $E_{ex}$ | 0.37 | 0.96 | 0.32 | 0.61 | 1.33 | 1.04 | 1.07 |

indication of a collective wave function extended into the plane of non-axial deformation.

Figure 5 shows the collective excitation spectrum for $I = 0$, 2 and 4 in $^{72}$Kr as a function of the angular momentum. We can see that the prolate and oblate states get close in energy at finite angular momentum. We have also plotted the experimental data [5] for the low spin states. The ground state is thought to be oblate but the rotational band built on top of it is thought to be prolate.

The second experimental $I = 0$ state is interpreted as the prolate band-head. Our calculations support these conclusions with the exception of the interpretation of the second 0-state. We find the prolate band head to be lower-lying in energy than seen in experiment and we also see very little mixing of the oblate and prolate states at $I = 0$. An alternative interpretation would be that the second 0-state is a spherical state in our calculation, since this state has a higher energy and a larger mixing with the oblate state.

In summary, we have extended the method of calculating the self-consistent collective path presented in [3, 11] to include constraints on angular momentum. We have been able to determine the collective coordinate from the Hamiltonian without having to assume a priori which are the relevant degrees of freedom. The results confirm the importance of pairing collapsed states for the collective path as suggested in Ref. [11]. We have also seen the effect of rotation on the collective path: Without rotation the path goes through a spherical saddle-point in contrast to the rotating case where the two minima are connected via the triaxial plane, and as we increase angular momentum the collective path disappears. The changes would probably be less pronounced if we would have allowed for more than one collective coordinate, which a calculation we intend to do in the near future. We have compared our calculations with experimental data [5] and found a reasonable agreement.

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