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YRAST BANDS AND HIGH-SPIN POTENTIAL-ENERGY SURFACES

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The yrast sequence of states for high angular momenta is studied. The modified-oscillator field with the inclusion of an ωJ_x term to describe the effects of nuclear rotation forms the basis for the calculation of microscopic energies. The macroscopic energies are provided by surface and Coulomb energies, and the rotational energy corresponding to rigid rotation.

In the deformed regions the "yrast" band squence of states for even-even nuclei is so far well established up to I of the order of $20\hbar$. The region of backbending occurs for I-values usually between 10 and $20\hbar$. In most cases it appears that backbending is associated with the decoupling or rotation alignment of specific orbitals [1]. The reduction in pairing seems to be significant but not dramatic in the beginning of the backbending region. All through this region the nucleus is usually stably prolate. However, as pointed out by Bohr and Mottelson [2], the decoupling mechanism obviously involves the breaking of axial symmetry. Detailed Bogolyubov type calculations in this region, e.g. those performed by Fässler [3], imply mean deformations into the gamma plane of 5–10° for $I \gtrsim 20\hbar$. The decoupling also implies a weakening in the pair correlation energy. Beyond 20–30 units of angular momentum the pair coupling scheme appears to have collapsed. The gamma transitions that precede the known yrast band appear to involve collective bands associated with triaxial rotors [2].

From liquid-drop calculations (with the drop rotating rigidly) Cohen, Plasil and Swiatecki [4] in 1973 predicted the following behaviour of the nuclear shape as a function of the rotational angular momentum. For $I=0$ the equilibrium shape of the uncharged liquid drop is obviously a sphere. For increasing I the sphere flattens at the poles, hereby increasing the moment of inertia. The inertia can then be increased additionally by a lifting of the axial symmetry. The equilibrium point thus moves into the gamma plane and ultimately the equilibrium shape degenerates into a needle prolate. This behaviour with I is expected to be significantly modified by the inclusion of shell structure. To the sum of liquid-drop and rigid rotational energy is to be added the shell correction energy, which latter is a function of the rotational frequency.

The basis of static ($I=0$) shell energy calculations is the assumed existence of a single-particle field

$$H_0 = \sum h_0 \,, \tag{1}$$

where

$$h_0 = -\frac{\hbar^2}{2m}\Delta + V \,, \tag{2}$$

with wave functions

$$h_0\phi_i = e_i\phi_i \,. \tag{3}$$

For $I \neq 0$ we have to add an auxiliary condition to the *generator* Hamiltonian

$$H_\omega = H_0 - \omega J_x = \sum h_\omega \,, \tag{4}$$

with

$$h_\omega = h_0 - \omega j_x \,, \tag{5}$$

where we thus assume that the rotation takes place around the x-axis, which for $0 < \gamma < 60°$ (apart from possible shell fluctuation) is the axis for which the inertia is maximum. Furthermore we assume that the quantum mechanical wobbling may be neglected for

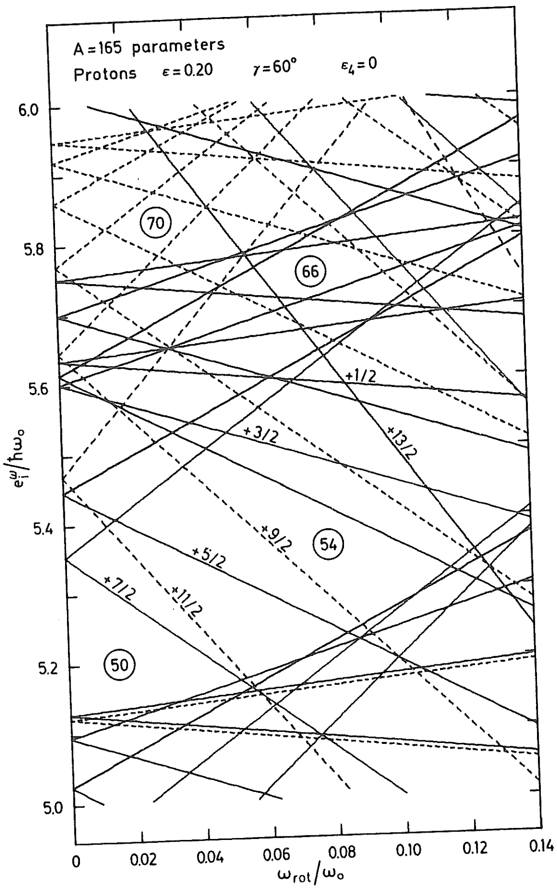

Fig. 1. Single-proton energies e^{ω} measured in the rotating system as functions of the rotation frequency ω. The figure refers to the pure oblate case $\epsilon = 0.20$, $\gamma = 60^{\circ}$ with the x-axis being the rotation and symmetry axis.

the high angular momenta in question.

One may also look at the Hamiltonian H_{ω} as the Hamiltonian in the rotating system. The ωJ_x term then takes the role of the Coriolis and centrifugal correction terms. Let us denote the corresponding single-particle energy e_i^{ω} and wave function ϕ_i^{ω}

$$h_{\omega}\phi_i^{\omega} = e_i^{\omega}\phi_i^{\omega} \ . \tag{6}$$

It is to be noted that for the rotating field the time-reversal degeneracy is broken (see fig. 1).

Each orbital is associated with an angular momentum expectation value

$$\langle m_i \rangle = \langle \phi_i^{\omega} | j_x | \phi_i^{\omega} \rangle \ . \tag{7}$$

Obviously $\langle m_i \rangle$ is not a constant of the motion and it need not be half-integer, except for the case of $\gamma = 60^{\circ}$.

For any given configuration the corresponding uncorrected energy is given as

$$E_{\rm sp} = \sum_i \langle \phi_i^{\omega} | h_0 | \phi_i^{\omega} \rangle = \sum_i \langle e_i \rangle \ , \tag{8}$$

where $\langle e_i \rangle$ obviously is not an eigenvalue. In fact we have

$$e_i^{\omega} = \langle e_i \rangle - \langle m_i \rangle \omega \ , \tag{9}$$

and

$$E_{\rm sp} = \sum e_i^{\omega} + \omega M \ , \tag{10}$$

where

$$I = M = \sum \langle m_i \rangle \ , \tag{11}$$

is the required total angular momentum.

Eq. (8) expresses a relation between the total energy and the rotational frequency ω, while the relation between I (or M) and ω is given by (11). Through (8) and (11) we may obtain the required relation between $E_{\rm sp}$ and I.

The difficulties encountered in the evaluation of the total energy through the summation of single-particle energies for the $I = 0$ case are present also in the $I \neq 0$ problem. As in the former case a successful resolution is provided by the use of the shell-correction method [5], which thus can be adapted also to the $I \neq 0$ case. We will here follow the formulation given by Jennings [6]. (Cf. also Badhuri and Ross [7], Brack [8] and Hamamoto [9].)

We define the level distribution functions in e^{ω} space:

$$g_1(e^{\omega}) = \int_{-\infty}^{\infty} \mathrm{d}m\, g(e^{\omega}, m) = \sum_i \delta(e^{\omega} - e_i^{\omega}) \ , \tag{12}$$

and correspondingly an angular-momentum density

$$g_2(e^{\omega}) = \int_{-\infty}^{\infty} m\, \mathrm{d}m\, g(e^{\omega}, m) = \sum_i \langle m_i \rangle\, \delta(e^{\omega} - e_i^{\omega}) \ , \tag{13}$$

starting from the two-dimensional level distribution in (m, e^{ω}) space. One can now obtain from the discrete distributions $g_1(e^{\omega})$ and $g_2(e^{\omega})$ the continuous ones $\tilde{g}_1(e^{\omega})$ and $\tilde{g}_2(e^{\omega})$ as e.g.

$$\tilde{g}_1(e^{\omega}) = \int_{-\infty}^{\infty} S(e^{\omega} - e_1^{\omega})\, g_1(e_1^{\omega})\, \mathrm{d}e_1^{\omega} \ , \tag{14}$$

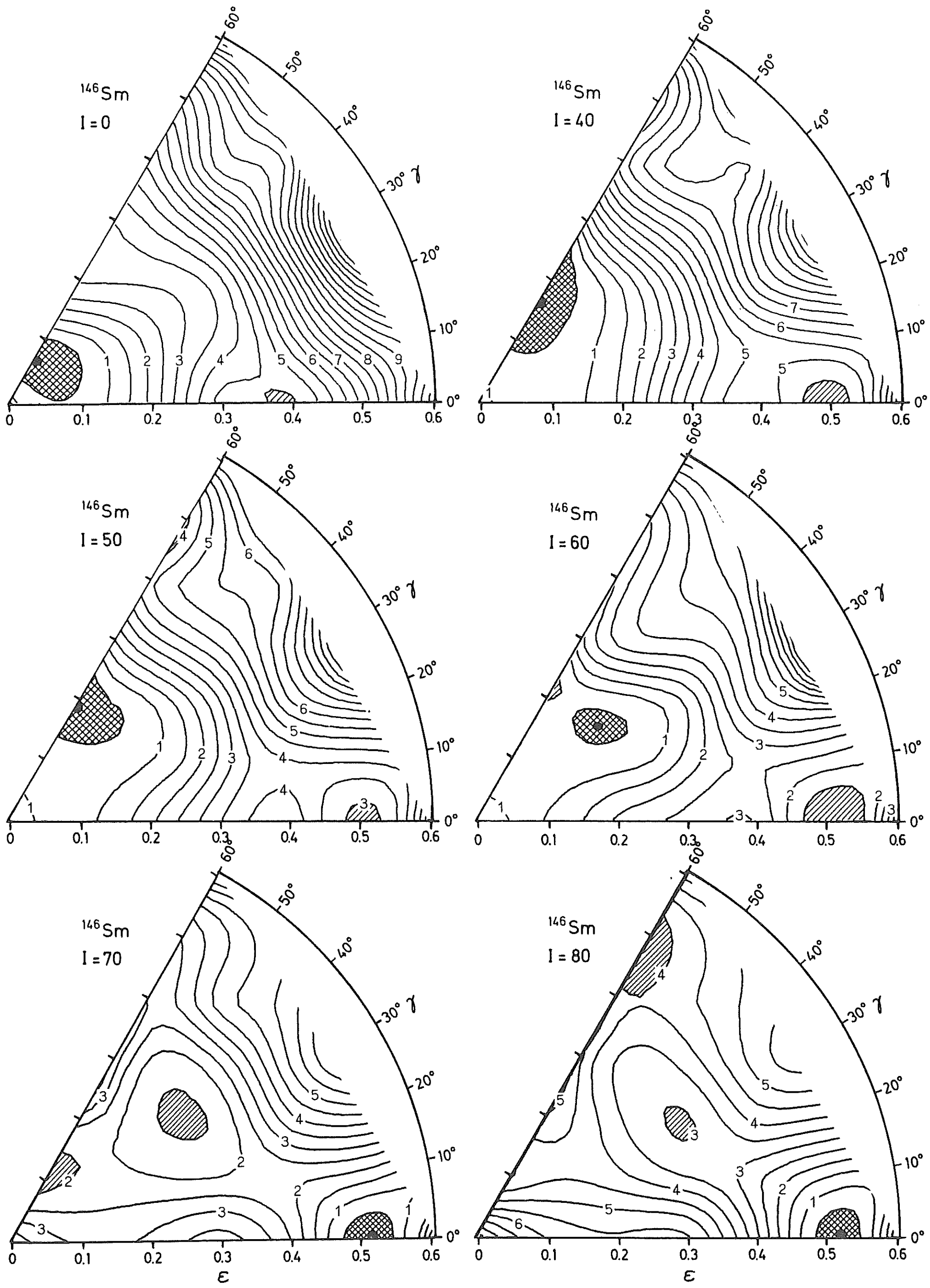

Fig. 2a–f. Total energy (and no pairing) for $^{146}_{62}$Sm for a) $I = 0$, b) $I = 40\hbar$, c) $I = 50\hbar$, d) $I = 60\hbar$, e) $I = 70\hbar$, f) $I = 80\hbar$. Cross shaded area marks ground-state minimum. Numbers on contour lines denote energy (in MeV) relative to the minimum point.

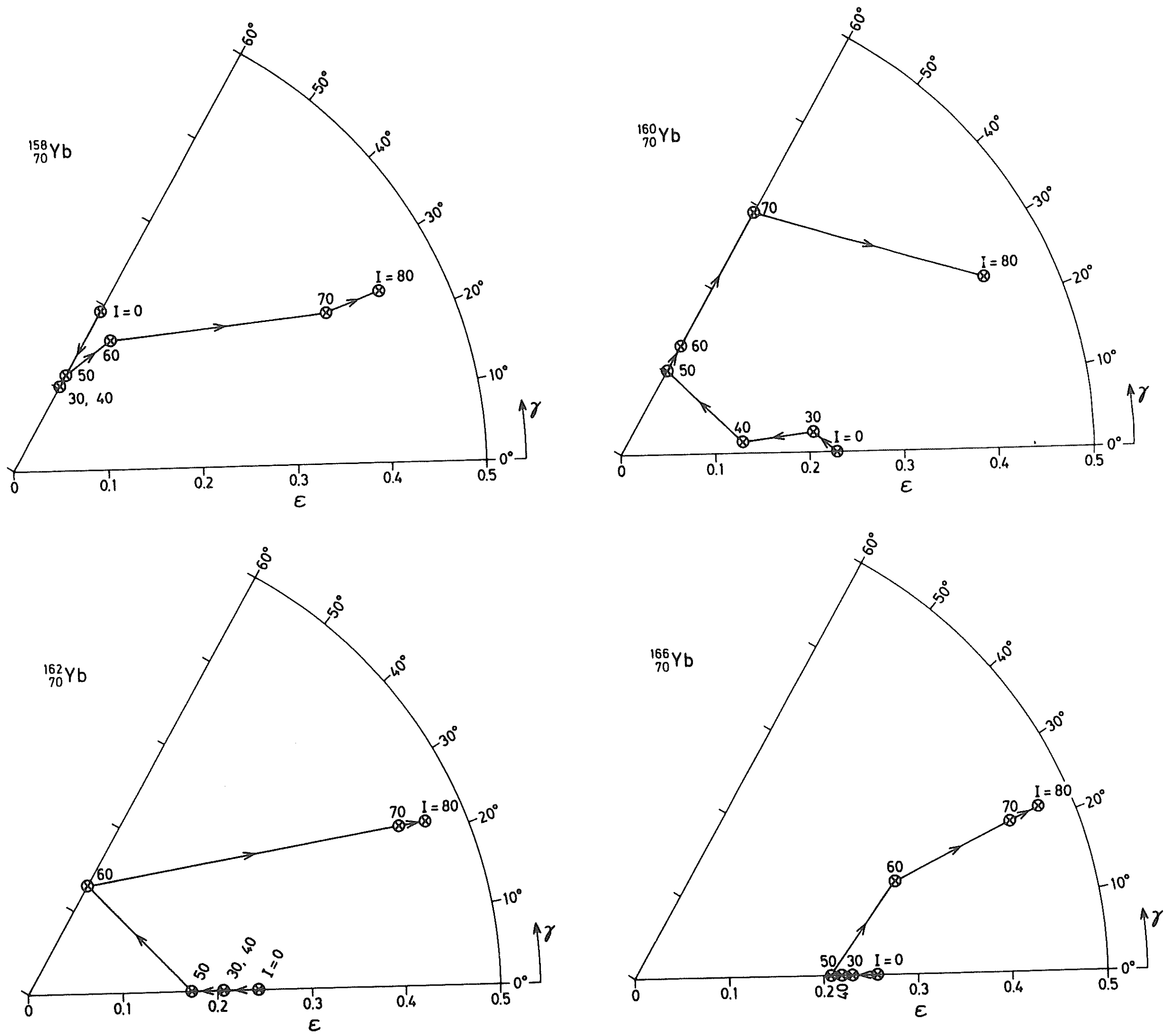

Fig. 3a–d. Sequence of deformations reached by the nuclei ^{158,160,162,166}Yb as functions of angular momenta.

where $S(e^{\omega} - e_1^{\omega})$ is the Strutinsky smearing function. Based on the sharp population of the unsmeared distributions we have

where $S(e^{\omega} - e_1^{\omega})$ is the Strutinsky smearing function. Based on the sharp population of the unsmeared distributions we have

$$I = M = \int_{-\infty}^{\lambda} g_2 \, \mathrm{d}e^{\omega} = \sum_i \langle m_i \rangle , \tag{15}$$

$$E_{\mathrm{sp}} = \int_{-\infty}^{\lambda} g_1 e^{\omega} \, \mathrm{d}e^{\omega} + \omega M = \sum_i e_i^{\omega} + \omega M . \tag{16}$$

For the smeared level distributions the corresponding equations transform into

$$I = M = \int_{-\infty}^{\widetilde{\lambda}} \widetilde{g}_2 \, \mathrm{d}e^{\omega} , \tag{17}$$

$$\widetilde{E} = \int_{-\infty}^{\widetilde{\lambda}} \widetilde{g}_1 e^{\omega} \, \mathrm{d}e^{\omega} + \widetilde{\omega} M , \tag{18}$$

The auxiliary quantities ω, $\widetilde{\omega}$, λ and $\widetilde{\lambda}$ are determined so as to obtain the quantities $E_{\mathrm{sp}}(I)$ and $\widetilde{E}(I)$, both defined for the same I. The difference $E_{\mathrm{sp}}(I) - \widetilde{E}(I)$

represents the shell-correction energy. The uncorrected energy E_{sp} includes the rotational energy. Similarly E_{shell} obviously includes *fluctuations* in the rotation energy. The quantity E_{shell} includes shell corrections both to the intrinsic and rotational energy. It is thus calculated as

$$E_{shell} = \sum e^{\omega} + \omega I - \widetilde{E} \;.$$

With the shell energy available for each I-value the total energy is obtained from the sum of the shell energy, the (rigid) rotational energy and the liquid-drop surface and Coulomb energies:

$$E(I) = E_{shell}(I) + E_{l.d.} + \frac{\hbar^2}{2J_{rig}} I^2 \,,$$

where J_{rig} is the rigid inertia for the shape defined by ϵ and γ (the principal value). It is to be noted that by this procedure we have replaced the smooth rotational energy obtained from $\widetilde{E}(I)$ by the smooth rotational energy corresponding to a rigid body of the same shape.

Technically, the calculation is carried out as follows. A set of ω-values in steps of 0.01 ω_0 from $\omega = 0$ to $\omega = 0.12\ \omega_0$ (where ω_0 is the oscillator frequency) is chosen, furthermore a set of grid points in the ϵ, γ plane. (As pointed out to us by Nergaard [10] it is important to go somewhat below 0° in the gamma plane, allowing for rotations around a principal axis with a moment of inertia classically smaller than the maximal one. However, the preliminary calculations reported here were confined to the $\gamma = 0$ to 60° sector of deformations.) For these grid points the shell energy is calculated for $\epsilon_4 = 0$ only, due to computer time limitations. However, for the rotational and liquid-drop energies an ϵ_4 variation was permitted so as to minimize the sum of liquid-drop and rotational energy.

Furthermore for each ω a value of I and E_{sp} is calculated from (11) and (8). As $\widetilde{E}$ is found to be a very smooth and almost linear function in I^2, $\widetilde{E}$ for any arbitrary I-value is readily obtained through an interpolation in I^2 between the calculated points.

In this way for each grid point in ϵ and γ a value of E_{shell} is obtained for a small number of I-values, which obviously are not the same for the different grid points. One of the major approximations in the calculation is then that values of E_{shell} for the final I-values, $I = 40$, 50, 60$\hbar$ etc., are obtained through interpolations from the calculated points, which latter correspond presently to, all in all, ten different ω-values.

A few of the results are summarized in figs. 2a–f and 3a–d. Thus in fig. 2a–e we exhibit a map in the ϵ, γ plane of $E(I)$ as a function of ϵ and γ for $I = 0, 40$, 50, 60, 70 and 80$\hbar$ for the neutron deficient nucleus ^{146}Sm, which is found to be favourable for the establishment of stable dynamical oblate shapes. In fig. 3a–d we give the loci of equilibrium shapes as a function of spin for the nuclei ^{158,160,162,166}Yb.

The simultaneous occurence of large negative shell energies and liquid-drop minima for certain values of ω (and corresponding I-values) opens the possibility of yrast traps connected with those spin values. However, this latter phenomenon requires a more detailed investigation. More complete results will be available in a forthcoming publication.

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