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DISCLAIMER

EXPONENTIAL DEPENDENCE OF THE NUCLEAR MOMENT-OF-INERTIA ON PAIRING CORRELATION AND THE PAIRING STRETCH MODEL FOR NUCLEAR ROTATION*

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ABSTRACT

Nuclear moments of inertia calculated from the cranking model show the dependence on pairing correlation to be nearly exponential over most of the region of physical interest. Furthermore, the uncorrelated wave functions yield moments-of-inertia deviating in some cases considerably from rigid body values. A two-dimensional pairing stretch model is developed and rotational energies are calculated up to spin 18 for five deformed nuclei. With two adjustable parameters the energy fits are quite good, but our calculations show neither pairing collapse nor "back-bending".

THE EXPONENTIAL DEPENDENCE

One of the central problems in the study of deformed nuclei is how to calculate the moment-of-inertia* J. It is now well-known that 1): The experimental value of J for the nuclear ground state lies between the rigid-body and irrotational flow limits, and it depends strongly on the nuclear pairing correlations;[1] 2): In the ground rotational band the value of J increases for increasing spin due to centrifugal stretching, Coriolis-anti-pairing, higher-order cranking, and other effects; 3): More recently the experimental discovery of back-bending[2] showed that some nuclei exhibit sharp, almost discontinuous increases in moment-of-inertia above a critical spin. In all cases the pairing correlation plays an important role. Hence, we shall restrict ourselves in this paper to the relation between pairing correlation and the moment-of-inertia and the application of these relationships to calculation of the rotational energies. We shall not attempt a comprehensive referencing to the extensive work in this field but refer the reader to a recent review article <u>Dependence of Moment-of-Inertia on Pairing</u>.[3]

The moment-of-inertia can be calculated using the well-known second-order cranking formula of Inglis[4] and Belyaev[5]

$$J = 2\hbar^2 \sum_{\Omega_\alpha > 0} \frac{|\langle \alpha' | j_x | \alpha \rangle|^2}{E_{\alpha'} + E_\alpha} (U_{\alpha'} V_\alpha - V_{\alpha'} U_\alpha)^2 \tag{1}$$

where $|\alpha\rangle$ is the single particle wave function with α representing the appropriate quantum numbers; Ω_α is the magnetic quantum number along the symmetry

*We shall use ordinary J for the moment-of-inertia, rather than the script letter in common usage. There should not be any confusion with angular momentum, for which the symbol I is used.

axis; U_α and V_α are the probability amplitudes of the orbital α in the presence of pairing; and E_α is the quasi-particle energy expressed by

$$E_\alpha = (\varepsilon_\alpha - \lambda)\,(U_\alpha^2 - V_\alpha^2) + 2U_\alpha V_\alpha G \sum_{k>0} U_k V_k \tag{2}$$

where ε_α is the single particle energy, λ is the chemical potential and G the pairing force strength. Following our previous treatment,[6] we parametrize U_α and V_α by introducing a pairing correlation parameter ν

$$\left.\begin{matrix} U_\alpha^2 \\ \\ V_\alpha^2 \end{matrix}\right\} = \frac{1}{2}\left[1 \pm \frac{\varepsilon_\alpha - \lambda}{\sqrt{(\varepsilon_\alpha - \lambda)^2 + \nu^2}}\right] \tag{3}$$

The quantity ν/G is the effective number of Nilsson orbitals participating in the pairing correlation. If $\nu = 0$, we have a sharp Fermi surface with no pairing correlation. If $\nu = \Delta$, where Δ is the pairing gap parameter, we have the BCS ground state, and Eq. (2) reduces to the usual BCS result, i.e.

$$E_\alpha = \sqrt{(\varepsilon_\alpha - \lambda)^2 + \nu^2} \qquad \text{for } \nu = \Delta \tag{4}$$

In what follows we shall vary the pairing correlation parameter ν for a given fixed pairing strength G to study the behavior of J as expressed by Eq. (1). Since for $\nu \neq \Delta$ the BCS gap equation no longer holds, Eq. (4) is not valid. It is thus important to use Eq. (2) rather than Eq. (4) for the energy denominators in the moment-of-inertia expression; they yield identical results only for the BCS ground state where $\nu = \Delta$.

We have carried out cranking model moment-of-inertia calculations for a range of ν values for rare-earth nuclei, and the results are plotted in Figs. 1 and 2 for protons and neutrons, respectively. In our present calculations the $|\alpha\rangle$ and ε_α are chosen to be the Nilsson functions and eigenvalues expanded across oscillator shells up to N = 12 for neutrons and N = 11 for protons, using computer programs derived from the 1969 work of Nilsson et al.[7] The quadrupole and hexadecapole deformation parameters ε and ε_4 for each nucleus were chosen equal to the theoretical values of Fig. 12a of Ref. 7 and were kept fixed while varying ν. The values of pairing-force strength were also taken from Ref. 7 as

$$G = \frac{1}{A}\left[g_0 \pm g_1 \frac{N - Z}{A}\right] \tag{5}$$

with plus sign for protons and minus sign for neutrons, and g_0 = 19.2 MeV, g_1 = 7.4 MeV. For calculations with $\nu \neq \Delta$, we have adjusted λ so that the particle number equation

$$\sum_{\alpha>0} 2V_\alpha^2 = N$$

is always satisfied, although the BCS gap equation is not.

A striking result of our calculations is the degree to which the calculated moments-of-inertia conform to an exponential dependence on the pairing correlation parameters ν_p and ν_n, as is evident in the excellent straight line behavior in the ℓnJ vs ν plots of Figs. 1 and 2. This exponential dependence is valid for a wide range of ν values above the lower limit ν_L which is about 20% - 30% of the energy gap Δ of the BCS ground state. For ν values smaller than ν_L there are usually some deviations. Thus, we can express the moment-of-inertia J as

$$J(\nu) = J^{(0)} e^{-\gamma\nu} \qquad \text{for } \nu_L \lesssim \nu \lesssim \Delta \tag{6a}$$

$$\frac{\nu_L}{\Delta} \sim 0.3 \tag{6b}$$

where $J^{(0)}$ is the $\nu = 0$ extrapolated value from the ℓn J vs. ν plot. The values of γ and $J^{(0)}$ for protons and neutrons of rare-earth nuclei can be extracted from Figs. 1 and 2 and are given in Table I. The deviation from the exponential dependence at small ν values does not limit the usefulness of Eq. (6). In fact, the region ($\nu_L \leqslant \nu \leqslant \Delta$) in which the exponential dependence holds usually covers the region of physical interest for most problems. For example, the pairing correlation decreases as one goes up the rotational band due to the Coriolis-anti-pairing effect, but our model calculations outlined later in this paper show that even for spin I = 18 corresponding to the rotational frequency near the Mottelson-Valatin limit,[8] the equilibrium value of $\nu(I = 18)$ will still be larger than ν_L.

It is interesting to note that the exponential dependence of the moment-of-inertia on pairing holds only for well deformed nuclei, which lie far from closed shells. As an example, the lnJ vs. ν plot of neutron and proton for several Pt isotopes is given in Fig. 3. In the case of neutrons, since their number is still far away from the magic number N = 126, the neutron moment of inertia continues to follow the exponential dependence very well. On the other hand, the proton number of Pt isotopes is close to the magic number Z = 82, and as a result, the proton plots are now no longer straight lines. In fact, the low-lying levels of Pt isotopes resemble more closely vibrational spectra.

We have also directly calculated the moment-of-inertia at zero pairing ($\nu = 0$) which we denoted as J_0. Note that in general J_0 does not equal the extrapolated value $J^{(0)}$. The difference between J_0 and $J^{(0)}$ is an indication of the degree of deviation from the exponential dependence at small ν. The resulting J_0 for several rare earth nuclei together with the corresponding rigid-body values are listed in Table II for comparison, where the rigid-body value is evaluated by

$$J_{rig} = \frac{2}{5} M A R^2 (1 + 0.33\ \varepsilon)$$

with $R = 1.2 \cdot A^{1/3}$ fm.

It is seen from Table II that there are often substantial deviations of J_0 from J_{rig}. It has been proved[1] that for nucleons moving in a pure anisotropic harmonic oscillator potential the moment-of-inertia of the system should be equal to the rigid-body value for the nucleus at its equilibrium deformation. Evidently, the spin-orbit term and the anharmonicity (ℓ^2 term) of the Nilsson potential cause the deviations, positive at the beginning of the deformed region and going negative with increasing mass, corresponding to the filling of the highest-j orbitals.* Thus, for realistic treatments one should not automatically assume that the moment-of-inertia goes to the rigid body limit after pairing correlation is lost. Furthermore, diagonal elements of the pairing interaction ($\overline{G}_{\nu\nu}$ in the notation of Belyaev)[5] can, by increasing energy denominators, reduce the cranking moment-of-inertia below our calculated values of a sharp Fermi surface.

*Our calculations are not carried out at the precise equilibrium deformation values in the absence of pairing. Rather are the equilibrium deformation values those of Nilsson et al.[7] calculated in the presence of pairing. The differences for these strongly deformed nuclei are not expected to be very significant.

Usually the calculations of moment of inertia are performed only in the region of physical interest where ν is less than the ground state pairing gap parameter Δ. We have, however, carried out the cranking calculations for ν values larger than Δ in a few cases and the results are given in Fig. 4. The $\ln J$ vs. $\ln\nu$ plot in Fig. 4 indicates that the moment-of-inertia for unphysically large values of pairing is better described by an inverse power dependence on pairing, rather than exponential. This result, however, is of no practical importance because there are no physical situations in which pairing would exceed its full strength at the ground state. Nevertheless the fact that the exponential pairing dependence of moment-of-inertia holds over most of the region of physical interest may be somewhat fortuitous.

TWO-DIMENSIONAL PAIRING STRETCH MODEL

It is now known[9] from multiple Coulomb excitation, from μ-mesic x-ray work, and from Mössbauer experiments that quadrupole shape stretching with rotation is quite small except for nuclei bordering the deformed region (i.e. N = 90, 92). Thus, the generalized-normal-coordinate stretch variable of the VMI (variable-moment-of-inertia) and other models (cf. Sec. III B of Ref. 6) is predominantly a pairing correlation coordinate for most deformed nuclei and is not much coupled to shape changes. Hence, our microscopic demonstration of the exponential dependence of J on ν provides support for Draper's[10] EXP modification of the VMI model.

It seemed of interest to proceed further to make a two-dimensional pairing modification of the Diamond, Stephens, Swiatecki stretch model.[11] Whereas their equation reads

$$E = \frac{\hbar^2}{6B\beta^2} I(I+1) + \frac{1}{2} C(\beta - \beta_0)^2 \quad , \tag{7}$$

we write an analogous equation in the two pairing coordinates ν_p and ν_n as:

$$E = \frac{\hbar^2}{2J(\nu_p,\nu_n)} I(I+1) + V_{PBCS}(\nu_p) + V_{PBCS}(\nu_n) \tag{8}$$

The kinetic energy term will now be expressed in the exponential form found by cranking. Although cranking calculations well reproduce the general trend of experimental moments-of-inertia, cranking moments and higher order correction terms do not agree quantitatively with experiment.[12] Thus, in applying the exponential relation of Eq. (6) we shall introduce two adjustable correction factors a and b to allow adjustment of the calculated constants J_{0p}, J_{0n}, γ_p and γ_n as given in Tables I and II. The moment-of-inertia in Eq. (8) now reads

$$J(\nu_p,\nu_n) = aJ_{0p} \exp(-b\gamma_p \nu_p) + aJ_{0n} \exp(-b\gamma_n \nu_n) \tag{9}$$

The two correction-factors a and b are fixed by essentially forcing our calculations to fit the $2^+ \to 0^+$ and $4^+ \to 2^+$ transition energies. It would be more consistent to use the extrapolated $J^{(0)}$ values rather than calculated zero-pairing J_o values. However, the differences are small in most cases since the ratios of neutron to proton moments are about the same.

The number-projected BCS energy that plays the role of potential energy is calculated in the continuous model (cf. Eq. (4.20) of Ref. 6) and has the form

$$V_{PBCS}(\nu) = \rho[-\mu(\mu^2 + \nu^2)^{1/2} + \nu^2 \sinh^{-1}\frac{\mu}{\nu} - G\,\rho\,\nu^2(\sinh^{-1}\frac{\mu}{\nu})^2 + \mu^2]$$

$$+ \frac{G\rho\nu}{2}\tan^{-1}\frac{\mu}{\nu} - \frac{G\rho\nu}{2}\frac{(\sinh^{-1}\frac{\mu}{\nu})^2}{\tan^{-1}\frac{\mu}{\nu}} + \frac{G\nu\,\mu}{8(\tan^{-1}\frac{\mu}{\nu})\quad(\mu^2 + \nu^2)} \tag{10}$$

Subscripts p and n have been suppressed in the above expression used for the proton system and the neutron system. The pairing force strength G is that of Eq. (5). The matrix elements connect orbitals over an energy range $\pm\mu$ centered on the chemical potential. In the present calculations the cut-off μ was chosen as 0.8 $\hbar\omega_0$ to correspond to the use of $\sqrt{15Z}$ or $\sqrt{15N}$ states above and below the Fermi levels in Nilsson et al.[7] The Nilsson orbital density per MeV is ρ, and it is determined by demanding that Belyaev's continuous model[5] limit of the BCS gap equation be satisfied for the experimental odd-even mass difference Δ

$$1 = G\,\rho\,\sinh^{-1}\frac{\mu}{\Delta} \tag{11}$$

These experimental Δ values were taken from Nemirovsky and Adamchuk.[13]

For rough estimates of the CAP effect the potential energy of Eq. (10) could be approximated by the harmonic form

$$V_{PBCS} \simeq \text{const} + \frac{1}{2}\,(2\rho + \frac{2}{\pi\Delta})(1 - \rho G)(\nu - \Delta)^2$$

However, we have used the full functional expression of Eq. (10) in our two-dimensional stretch calculation. The Berkeley minimum search routine MINSER was used to find the minimum of the energy function (8) for successive even values of spin.

These calculations were carried out for five well-deformed nuclei $^{162}_{66}Dy$, $^{168}_{68}Er$, $^{172}_{70}Yb$, $^{178}_{72}Hf$, and $^{182}_{74}W$. Table III summarizes the results for rotational transition energies, comparing both with experiment and with the 3-parameter, "extended-VMI model" χ^2 fits of Saethre et al.[14] In general, our 2-parameter model calculations agree as well with experiment as the 3-parameter extended VMI (variable moment-of-inertia) model χ^2 fits of Saethre et al.[14] However, we get a more rapid increase of apparent moment-of-inertia at high spin than extended VMI, though we do not get "back-bending".

For the stretch model calculations of Table III the values of parameters a and b in Eq. (9) are summarized in Table IV. Note that the a parameters are close to 0.61 except for ^{182}W. That is, the cranking moments-of-inertia at zero pairing have to be further decreased in order that the rotors be stiff enough to match experiment. This reduction was necessary in spite of the fact that the values of J_0 were already less than rigid-body except for ^{162}Dy. It is tempting to suggest that diagonal pairing matrix elements $\overline{G}$ are involved in the reduction, but the lowest order cranking model cannot really be trusted quantitatively at very high angular momenta, and one must reserve judgment on diagonal pairing effects until much more sophisticated calculations have been done. In that connection the calculations with

Hartree-Fock-Bogoliubov theory and particle number projection are encouraging. Such calculations of Faessler et al.[15] also have angular momentum projection and avoid the cranking model. However, their constraint that the ratio of neutron and proton pairing remains constant is probably unrealistic, as our Table V brings out. In all cases the neutron pairing drops faster than proton pairing.

We note that in no case has there been a pairing collapse. The reason that pairing collapse does not occur here up to spins above the Mottelson-Valatin limit may be mainly due to our inclusion of a particle-number projection term in the pairing energy. Such projection always stabilizes pairing.

Though the stretch-model calculations presented here are not sufficiently sophisticated to be trustworthy at high spin, we hope that the physical insights of this model will be of value as a guide to future calculations on the challenging problem of nuclear rotational moment-of-inertia.

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Table I. The Extrapolated Values of Cranking Moment-of-Inertia At Zero Pairing and the Exponential Pairing Coefficient, See Eq. (6). [All Units in MeV^{-1}].

Nucleus	A	$\frac{2J_p^{(0)}}{\hbar^2}$	$\frac{2J_n^{(0)}}{\hbar^2}$	γ_p	γ_n
$_{62}Sm$	152	65.37	113.30	1.43	1.58
	154	64.43	134.29	1.28	1.52
	156	62.80	99.98	1.27	1.22
$_{64}Gd$	154	57.97	111.05	1.35	1.59
	156	60.04	132.95	1.29	1.54
	158	61.56	101.49	1.30	1.26
	160	62.80	102.51	1.32	1.14
	162	64.07	109.95	1.35	1.33
$_{66}Dy$	158	65.04	127.74	1.44	1.58
	160	65.04	103.54	1.40	1.32
	162	61.56	102.51	1.33	1.29
	164	62.18	109.95	1.36	1.36
	166	62.18	83.10	1.38	1.06
	168	62.80	90.02	1.41	1.15
$_{68}Er$	162	47.70	107.23	1.17	1.40
	164	46.99	101.49	1.13	1.31
	166	47.23	114.43	1.11	1.44
	168	46.06	83.10	1.06	1.05
	170	45.60	90.47	1.05	1.15
	172	45.60	88.68	1.05	1.18

(continued)

Table I. (cont.)

Nucleus	A	$\frac{2J_p^{(0)}}{\hbar^2}$	$\frac{2J_n^{(0)}}{\hbar^2}$	γ_p	γ_n
$_{70}Yb$	166	46.99	102.51	1.20	1.36
	168	48.42	116.75	1.19	1.47
	170	47.94	85.63	1.14	1.11
	172	47.94	93.22	1.11	1.20
	174	47.70	90.92	1.10	1.23
	176	48.42	67.36	1.12	0.89
$_{72}Hf$	174	35.52	90.92	0.95	1.19
	176	33.95	98.49	0.90	1.29
	178	33.45	72.97	0.90	1.05
	180	32.95	61.56	0.88	0.81
$_{74}W$	180	23.10	79.84	0.72	1.17
	182	23.10	62.80	0.71	0.83
	184	24.29	60.95	0.80	0.92
	186	25.79	54.60	0.94	1.01
$_{76}Os$	184	20.29	71.52	0.70	1.06
	186	21.12	64.07	0.76	1.04
	188	22.20	56.26	0.86	1.11

Table II. Cranking Moments-of-Inertia With No Pairing (All Units in MeV^{-1})

Z	A	$\left(\frac{2J_0}{\hbar^2}\right)_p$	$\left(\frac{2J_0}{\hbar^2}\right)_n$	$\left(\frac{2J_0}{\hbar^2}\right)_{total}$	$\left(\frac{2J}{\hbar^2}\right)_{rigid}$
66	162	60.22	102.68	162.90	143.96
68	168	40.98	76.39	117.37	153.66
70	172	40.65	82.38	123.03	159.66
72	178	38.05	76.30	114.35	168.12
74	182	22.03	55.73	77.76	173.49

Table III. Ground Band Transition Energies $E_I - E_{I-2}$ (keV)

Nucleus	I	This Calculation	Extended VMI 3-parameter χ^2	Experimental
$^{162}_{66}Dy$	2	80.70	80.660	80.660
	4	185.16	185.005	185.005
	6	282.72	282.865	282.864
	8	370.96	372.9	372.6
	10	448.78	455.4	453.7
	12	516.09	530.9	526.2
	14	573.44	600.5	
		621.67		
$^{168}_{68}Er$	2	79.80	79.7994	79.7998
	4	184.50	184.283	184.281
	6	285.27	284.634	284.646
	8	380.40	379.545	379.536
	10	468.67	468.5	
	12	549.37	551.7	
	14	622.20		
	16	687.10		
	18	744.15		
$^{172}_{70}Yb$	2	78.73	78.74	78.74
	4	181.57	181.52	181.52
	6	279.57	279.74	279.74
	8	370.72	372.2	371.9
	10	453.74	458.9	444.9
	12	528.00	540.2	498.0
	14	593.38	616.9	
	16	650.01	689.9	
	18	698.12		

(continued)

Table III. (continued)

Nucleus	I	This Calculation	Extended VMI 3-parameter χ^2	Experimental
$^{178}_{72}Hf$	2	93.20	93.118	93.181
	4	213.63	213.503	213.444
	6	325.62	325.533	325.562
	8	426.12	426.377	426.371
	10	513.60	515.2	
	12	587.69	592.7	
	14	648.69		
	16	697.04		
	18	732.70		
$^{182}_{74}W$	2	100.09	100.104	100.102
	4	229.34	229.323	229.317
	6	349.29	350.69	351.02
	8	456.65	464.1	464.0
	10	549.80	571.5	567.6
	12	628.41	676.4	

Table IV. Parameters a and b for Best Fits

Z	A	a	b
66	162	0.61	0.80
68	168	0.60	0.72
70	172	0.62	0.75
72	178	0.625	0.98
74	182	0.76	1.25

Table V. Calculated Gap Parameters

Nucleus	Spin I	Gap Parameters (MeV) $\Delta_p(I)$	$\Delta_n(I)$	$\Delta_p(I)/\Delta_n(I)$
$^{162}_{66}Dy$	0	0.879	0.989	0.89
	6	0.826	0.917	0.90
	12	0.715	0.760	0.94
	18	0.596	0.564	1.06
$^{168}_{68}Er$	0	0.933	0.774	1.21
	6	0.902	0.715	1.26
	12	0.832	0.576	1.44
	18	0.751	0.385	1.95
$^{172}_{70}Yb$	0	0.785	0.800	0.98
	6	0.750	0.736	1.02
	12	0.676	0.587	1.15
	18	0.597	0.386	1.55
$^{178}_{72}Hf$	0	0.969	0.753	1.29
	6	0.932	0.666	1.40
	12	0.864	0.474	1.82
	18	0.812	0.220	3.69
$^{182}_{74}W$	0	0.585	0.734	0.80
	6	0.543	0.645	0.84
	12	0.467	0.448	1.04
	18	0.410	0.183	2.24

Figure Captions

Fig. 1. This plot illustrates for proton systems of deformed nuclei the near-exponential dependence of theoretical cranking moments-of-inertia on pairing. The logarithm of the calculated moment-of-inertia is plotted vs. the pairing correlation parameter ν (particle number and pairing strength G held constant). The points are theoretical calculations with no reference to experiment.

Fig. 2. Same as Fig. 1 except for neutron systems.

Fig. 3. Same as Fig. 1 except that calculation is made on transitional platinum nuclei. Large deviations from exponential behavior are to be noted for the proton systems.

Fig. 4. The lnJ vs. lnν plot for ^{160}Dy and ^{174}Hf in region where the pairing correlation parameter ν is larger than the ground state pairing gap parameter Δ; p stands for proton and n for neutron. The straight portions indicate an inverse power dependence slightly greater than first power. Note deviations at both high and low pairing limits.

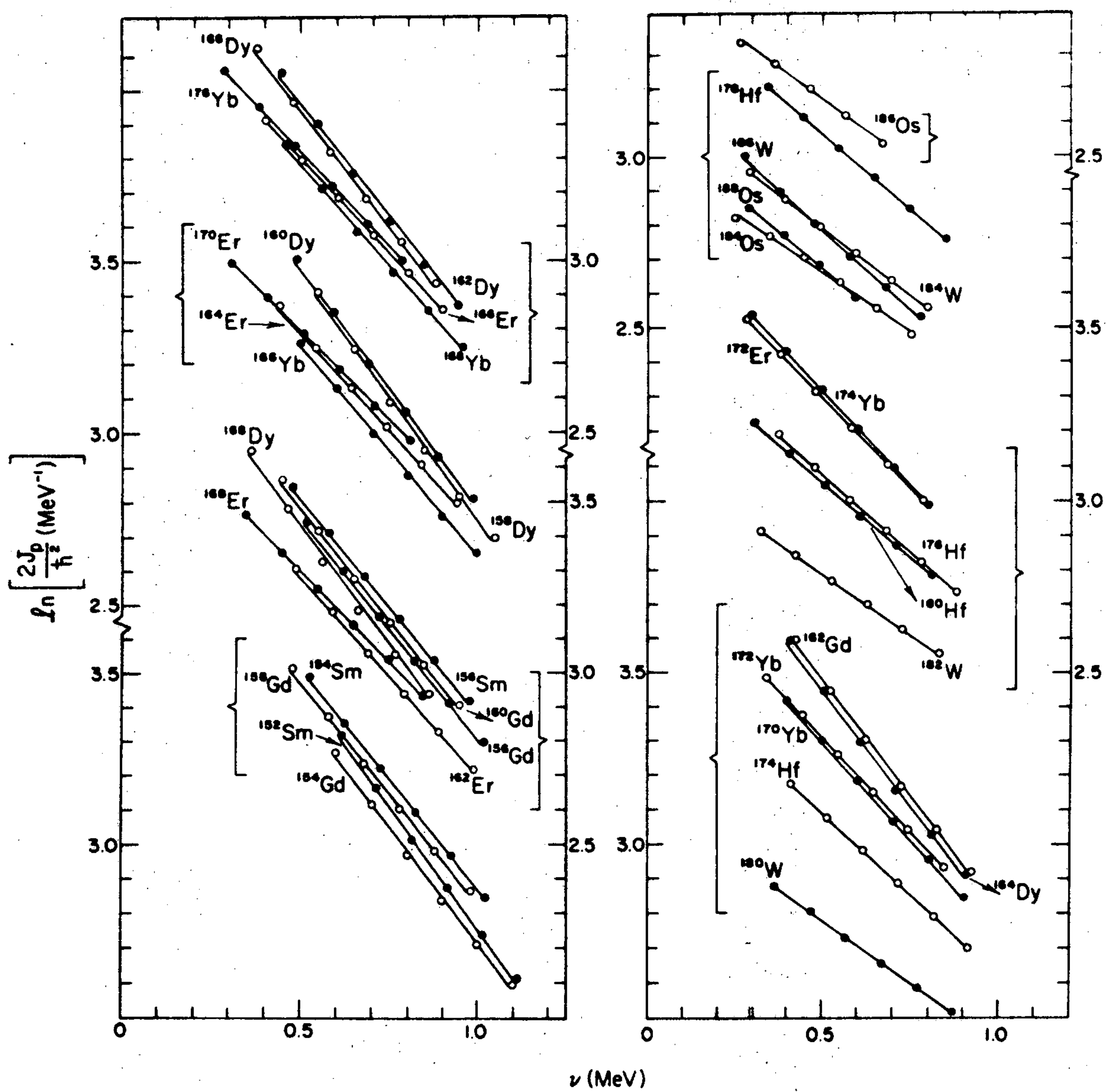

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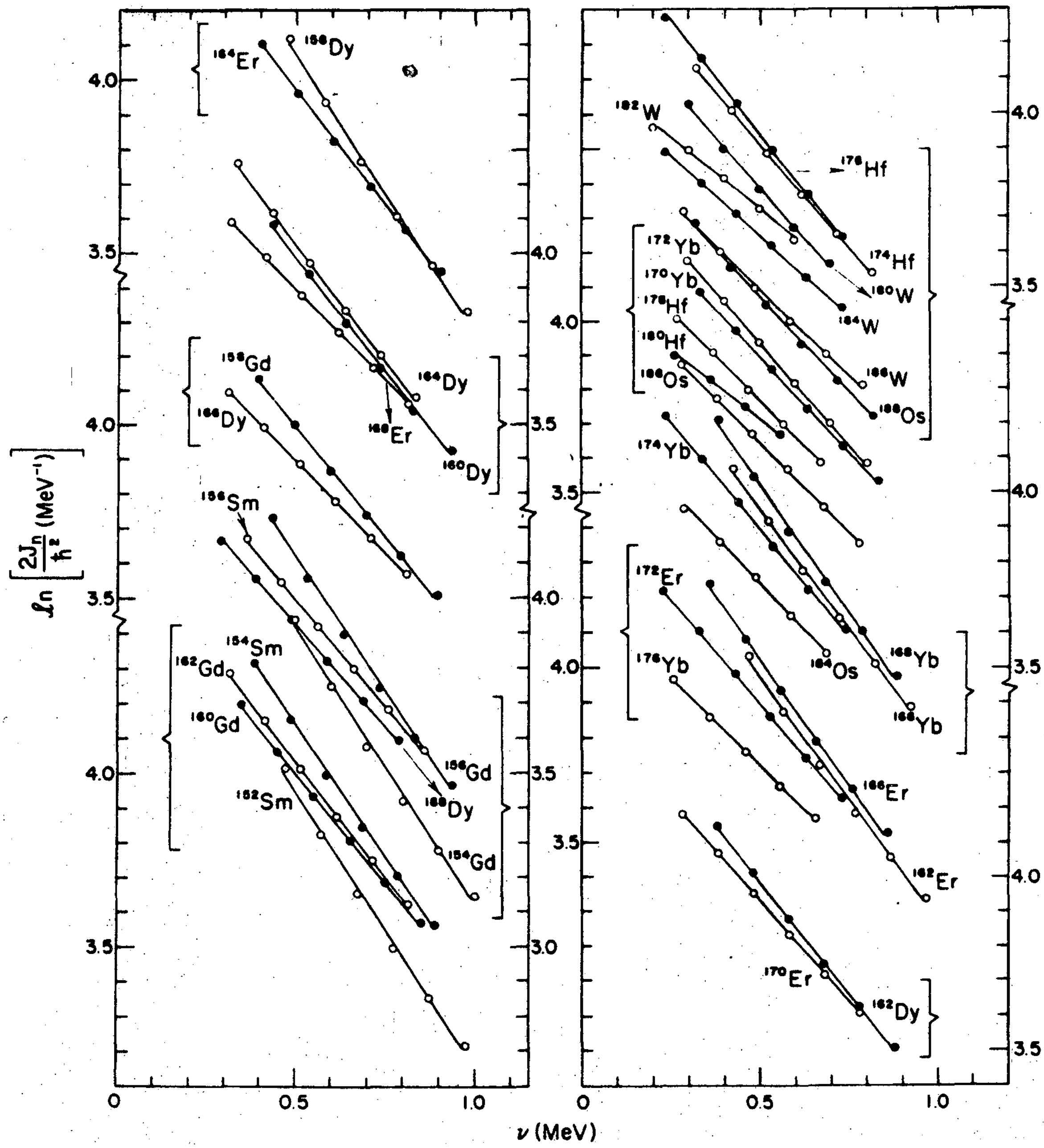
Fig. 1



$\ell n\left[\frac{2J_n}{\hbar^2}(MeV^{-1})\right]$
ν (MeV)
164Er
158Dy
164Dy
168Er
160Dy
158Gd
166Dy
156Sm
154Sm
162Gd
160Gd
152Sm
156Gd
168Dy
154Gd
162W
176Hf
174Hf
180W
184W
186W
188Os
172Yb
170Yb
178Hf
180Hf
186Os
174Yb
172Er
176Yb
184Os
168Yb
166Yb
166Er
162Er
170Er
162Dy
XBL 736-829

Fig. 2

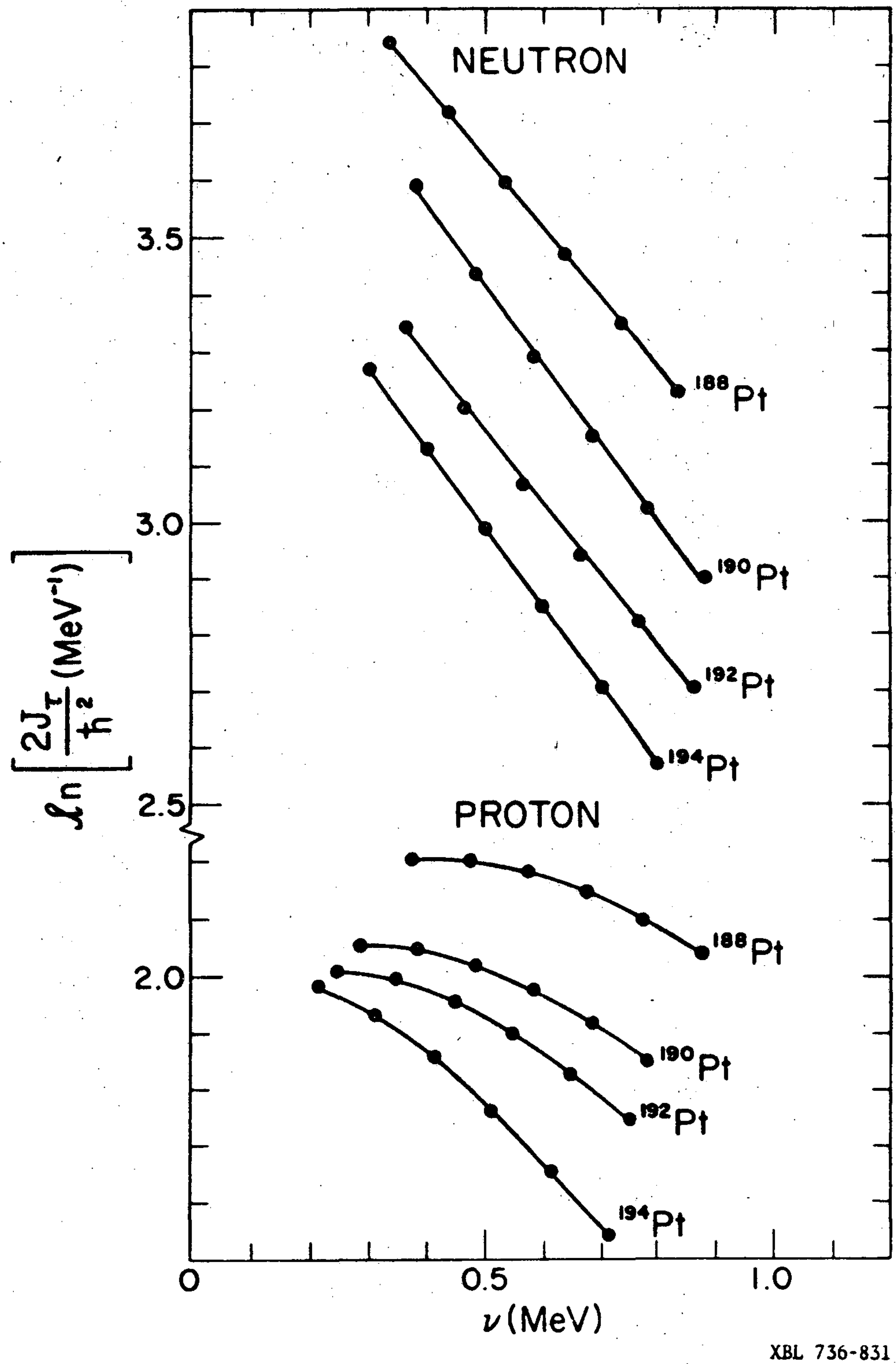

NEUTRON
PROTON
188Pt
190Pt
192Pt
194Pt
188Pt
190Pt
192Pt
194Pt
3.5
3.0
2.5
2.0
0
0.5
1.0
ν (MeV)
ln [2J_τ/ħ² (MeV⁻¹)]
XBL 736-831

Fig. 3

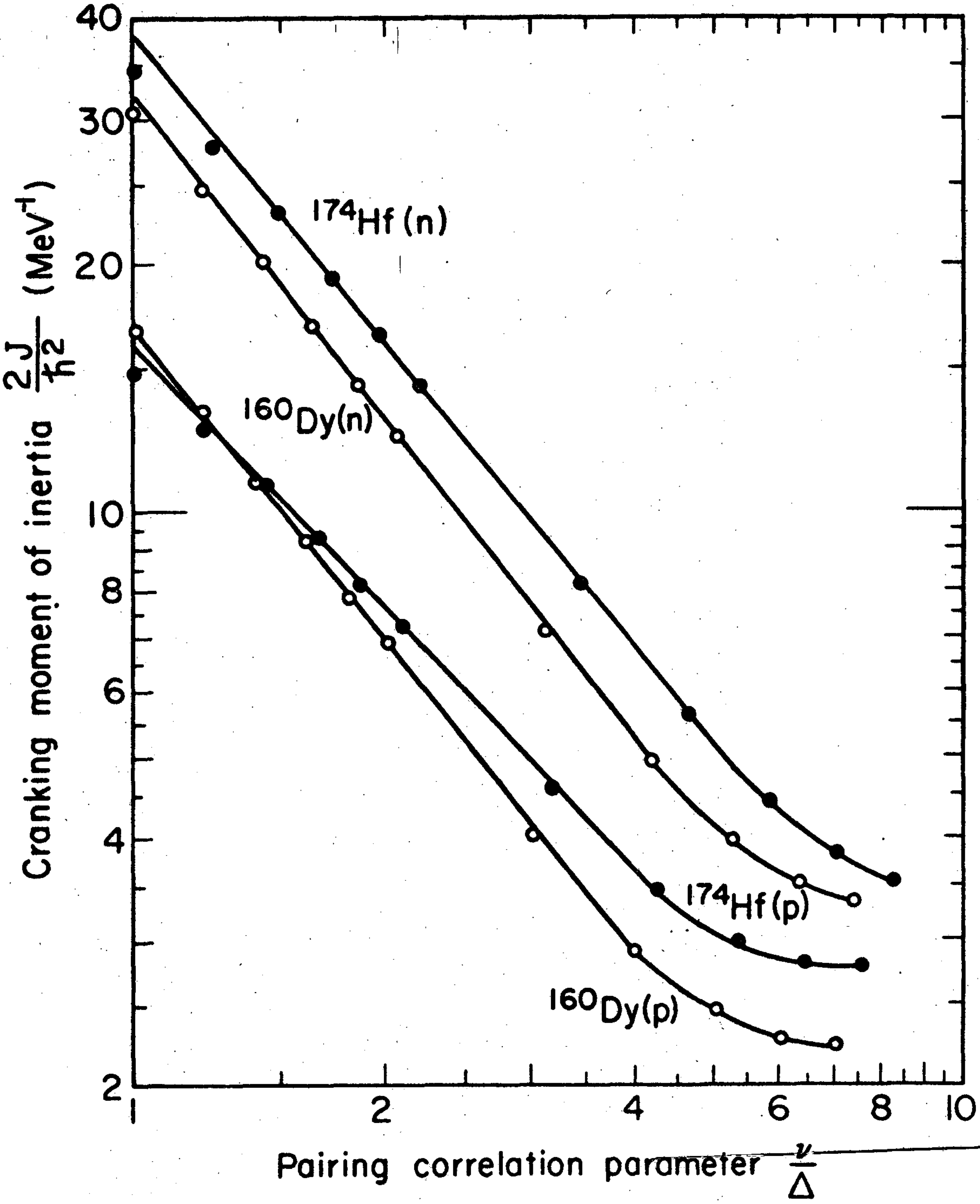

40
30
20
10
8
6
4
2
Cranking moment of inertia $\frac{2J}{\hbar^2}$ (MeV^{-1})
^{174}Hf (n)
^{160}Dy(n)
^{174}Hf(p)
^{160}Dy(p)
1
2
4
6
8
10
Pairing correlation parameter $\frac{\nu}{\Delta}$
XBL736-3191

Fig. 4