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Constrained–Hartree-Bogolyubov Treatment of the Pairing-Plus-Quadrupole Model: Discontinuities in Nuclear Moments at High Spins*

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I discuss a self-consistent, microscopic theory of nuclear rotations at high spins and review results obtained previously for the spin dependence of the moment of inertia, deformation, and energy gaps of ^{160}Dy. Additional results given here suggest some striking discontinuities in isomer shifts, gyromagnetic ratios, and $B(E2)$ values at high spins. Theoretical results are consistent with the recent measurements of gyromagnetic ratios and $B(E2)$ values, but a greater precision is needed to test the predicted discontinuities.

The backbending phenomenon at high spins, observed[1] in the energy-level spectra of deformed, even-even nuclei with $A = 158-168$, has renewed the interest of nuclear physicists in the problem of rotational-type states. The sudden decrease in the spacing of I and $I-2$ levels in a rotational-type spectrum ($I = 0, 2, 4, \ldots$ levels whose level spacing increases with I) at $I \sim 16$ is somewhat[2] surprising from the point of view of the collective model. On the other hand, it is quite surprising that one can talk about collective, rotational-type states at excitation energies of 3–4 MeV. According to the conventional picture of heavy, even-even nuclei, the two-quasiparticle states should start at about 2 MeV and many other noncollective states should become prominent at 3–4 MeV. The lack of observation of the expected high density of states is an unsolved puzzle.

Many nuclear physicists are now engaged in attempting to fit the observed energy spectra (for recent reviews, see papers by Johnson and Szymański, and Sorensen[3]). It is already clear that the backbending type of effect can be reproduced at least qualitatively in a variety of ways. Hence, it is obvious that we need to study the behavior of various nuclear moments [for instance, $B(E2)$ values, gyromagnetic ratios, isomer shifts, and particle-transfer amplitudes] at high spins in order to discriminate between the different models.

The main purpose of the present note is to provide semiquantitative estimates of the behavior of nuclear moments at high spins. Although such measurements are at present extremely difficult, they are already being attempted. Comparison with the available data on $B(E2)$ values[4] up to $I = 18$ and with the gyromagnetic ratios[5] up to $I = 10$ will be given.

Several microscopic treatments of nuclear rotations at high spins of heavy nuclei have been developed: the Nilsson model plus pairing and cranking,[6] the Nilsson-Strutinsky model plus pairing and cranking,[7] the pairing-plus-quadrupole (PPQ) model combined with generalized Hartree-Fock,[8] the PPQ model with Hartree-Fock-Bogolyubov (HFB) and cranking,[9] the PPQ model with HFB and projection techniques,[10] the PPQ model with constrained Hartree-Bogolyubov (CHB),[11] and the particles-plus-rotor models.[12] These methods have been compared in the excellent review article of Sorensen.[3]

The three main steps of the present method[11] (PPQ model with CHB) are the following: (i) A transformation is made from a spherical, single-particle basis to a deformed, single-particle basis. The transformation coefficients are determined by diagonalizing the average part of the two-body quadrupole force, $-DQ = -X\langle Q\rangle Q$, where X is the strength of the quadrupole force (same for p-p, n-n, and n-p) and $Q = r^2 Y_2$ is the quadrupole operator. The usual Hartree-Fock method would consist of an iterative procedure for solving the self-consistency condition $D = X\langle Q\rangle$. We accomplish the *same* purpose[13,14] in a much simpler way by treating D (or equivalently, $\beta = D/m\omega_0^2$, where m is the nucleon mass and ω_0 the oscillator frequency associated with the spherical basis) as a variational parameter of the theory. At the extrema of the potential-energy function $[V(D) = \langle D|H|D\rangle$, where H is the PPQ model Hamiltonian], the self-consistency condition $D = X\langle Q\rangle$ is satisfied automatically.[15] Our method of generating the deformed basis is as simple as in the calculations based on the Nilsson model,[6,7] but is as close to first principles as the enormously more complicated iterative procedure.[9,10,16]

(ii) A Bogolyubov transformation is made from the basis of step (i) to a deformed-quasiparticle basis. The u, v factors, which define this transformation, depend on the energy gap Δ and the Fermi energy λ in the usual way. The value of λ is determined by the constraint on the particle number, $\langle\hat{N}\rangle = N$. The energy gap Δ is treated as a variational parameter of the theory *instead* of solving the usual gap equation of the BCS theory. Transformations for neutron and proton states are independent. Hence, we have two independent variational parameters, Δ_p and Δ_n.

(iii) The expectation value of the two-body Hamiltonian H is minimized with respect to the three variational parameters of the theory—β, Δ_p, and Δ_n—*and* with respect to a constraint $\langle J_x\rangle = [I(I+1)]^{1/2}$, where J_x is the x component of the nuclear angular-momentum operator. Such a constraint requires the consideration of the modified Hamiltonian $H' = H - \omega J_x$, where ω is a Lagrange multiplier (which can be identified with the rotational frequency), and of the mixing between zero- and two-quasiparticle states caused by $-\omega J_x$. In the case of a general, two-body interaction, the determination of the mixing coefficients requires the solution of some complicated, nonlinear equations given by Thouless and Valatin.[17] However, this task is greatly simplified in the case of a separable, two-body interaction such as that of the PPQ model. In fact, unless one wishes to calculate the electromagnetic moments to higher orders, it is not necessary to evaluate these mixing coefficients explicitly. To the same degree of approximation as in the Thouless-Valatin theory, the expectation value of the PPQ Hamiltonian is given by

$$W_0(\beta, \Delta_p, \Delta_n) = V_0(\beta, \Delta_p, \Delta_n) + \frac{\hbar^2 I(I+1)}{2\mathcal{J}_0(\beta, \Delta_p, \Delta_n)}, \quad (1)$$

where the subscript 0 means that we are considering the lowest intrinsic state, V is the uncorrected expectation value of H, and the second term represents the correction due to constraint on angular momentum. Expressions for V and $\mathcal{J}$ have been given previously[13,14] (that for V has to be modified somewhat because the usual gap equation is not used).

Although the energy expression of Eq. (1) looks like the sum of a potential energy V and a rotational energy, where the moment of inertia $\mathcal{J}$ is given by the cranking model, there are several conceptual and practical differences.[11,18]

The usual constraint on the number of particles, $\langle\hat{N}\rangle = N$, has been included in the present calculation. It has been emphasized[3,9,10] that particle-number fluctuations, $\langle(\hat{N} - N)^2\rangle$, become large as $\Delta \to 0$. This would seem to require an additional constraint on $\langle\hat{N}^2\rangle$. However, this effect is not quite as serious in our method as in the method of Mang and co-workers.[9] They find that they need to include the additional constraint in order to obtain backbending at high spins. We obtain this effect in ^{160}Dy (see Ref. 11 and the results discussed below) without including this additional constraint. Undoubtedly, it would be better to include the additional constraint in future calculations of the present type.

All the parameters of the present calculation are exactly the same as those of our previous[14] calculation of the ground-state shapes of 82 rare-earth nuclei, except for two. One of them is the strength of neutron-pairing force (the ratio to the proton-pairing force is kept the same as before). It had to be increased by 10% in order to avoid the occurrence of backbending at $I = 12$. This increase of pairing constants reduced the calculated moment of inertia. Hence, it was necessary to increase the "core contribution" parameter B_C by a factor of 1.72. (When the additional constraint on $\langle\hat{N}^2\rangle$ is taken into account, these two changes will probably become unnecessary.)

The main results of the present study of ^{160}Dy (some of which are given in Ref. 11) are summarized below. (1) The calculated energy-level spacings of ^{160}Dy agree with experiment[1] up to $I = 14$ within 5 keV. (2) The calculated moment of inertia increases suddenly at $I_C = 16$, in agreement with experiment.[1] The calculated phase transition is somewhat too fast and indicates the need for including the additional constraint on $\langle\hat{N}^2\rangle$ discussed above. (3) The theory is capable of giving a backbending effect in an $\mathcal{J}$-versus-ω^2

plot.[1] (4) The sudden increase of $\mathscr{G}$ at $I_C=16$ is caused by the vanishing of neutron pairing ($\Delta_n \to 0$). This result agrees with the prediction of Chan and Valatin.[6] (5) The energy gap Δ_p decreases by 19% at $I=0$–16, but *increases* by 18% at $I=16\to 18$. The results (4) and (5) can be tested experimentally by measuring the amplitude for transferring two nucleons from the I state of nucleus A to the I state of nucleus $A+2$ (or $A-2$). Such experiments are in progress.[5] (6) The deformation β increases by 15% at $I=0$–16, but *decreases* by 12% at $I=16\to 18$.

(7) The contribution of the potential (V) term of Eq. (1) to the total spacing of I and $I+2$ levels is <30% below $I=16$, but is twice as large as $I=16\to 18$. The increase in $\mathscr{G}$ is so large that had it not been for the V term, the $I=18$ level would have been *below* the $I=16$ level. The V term is also responsible for the "peculiar" behavior of β and Δ_p at $I=16\to 18$. (8) The charge isomer shift, $[\langle I|r^2|I\rangle - \langle 0|r^2|0\rangle]/\langle 0|r^2|0\rangle$, increases from 6.6×10^{-5} for $I=2$ to 1.2×10^{-3} for $I=16$ but decreases to negative values for $I>16$. (9) The intrinsic quadrupole moment, $Q_I=\langle I|r^2Y_{20}|I\rangle$, increases by 11% at $I=0$–16, but decreases by 8% at $I=16\to 18$.

(10) The intrinsic gyromagnetic ratio decreases from 0.31 ($I=0$) to 0.20 ($I=16$) and becomes negative (−0.006) at $I>16$. Part of the decrease is due to the rapid decrease of Δ_n (or increase of $\mathscr{G}_n$) as pointed out by Sano and Wakai.[8] But a substantial part of the decrease, especially the negative value, comes from the so-called "spin-contribution" due to the $(g_s-g_l)\vec{s}$ part of the magnetic moment operator. Kalish, Herskind, and Hagemann[5] have measured the g value of ^{158}Dy to be 0.36 ± 0.06 for $I\leq 8$. No value is given for $I=10$, but a drop in the g value for $I=10$ is suggested.

(11) Comparison with the $B(E2)$ values of Ward *et al.*[4] is given in Fig. 1. Theoretical values have been obtained by combining the relation

$$\frac{B(E2;I\to I-2)}{B_{\mathrm{ROT}}(E2;I\to I-2)}=\left(\frac{Q_I+Q_I-2}{Q_2+Q_0}\right)^2, \qquad (2)$$

with the calculated values of Q_I discussed above. The relation (2) is based on the assumption that deviations from the rotational model (Q independent of I) are small.

As pointed out by Ward *et al.*, the conventional theory predicts a sudden drop in $B(E2)$ in the region of a superfluid ($\Delta\neq 0$) to normal ($\Delta=0$) phase transition. The present theory predicts a drop of only 8%, which is quite consistent with the experimental results.

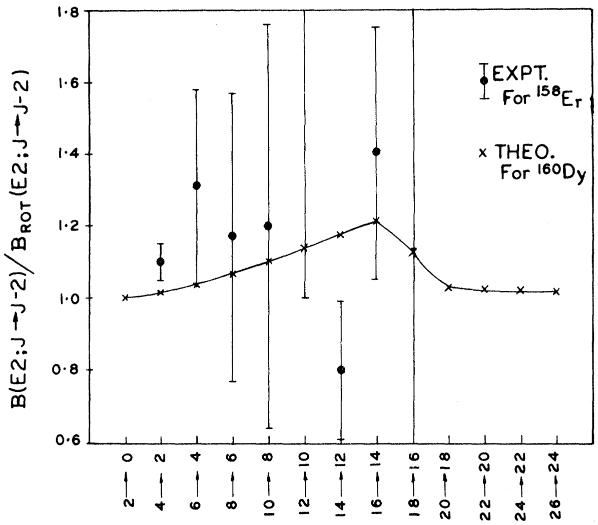

FIG. 1. Comparison of calculated with experimental $B(E2)$ values (see Ref. 4) ^{158}Er. Note that the phase transition occurs at $I=12$–14 in ^{158}Er but at $I=16$–18 in ^{160}Dy.

The main conclusion is that if our basic picture of the backbending effect (which is the same as the Mottelson-Valatin one[2,6-10] except for the fact that the shell effects are treated in a more complete way) is correct, then we should expect discontinuities in not only the energy spectrum but also in many nuclear moments. The available experiments provide partial confirmation, but are unable to discriminate between this picture and that of Stephens and Simon,[12] in which Δ remains unchanged and the backbending is caused by the decoupling of a single pair of neutrons in the $i_{13/2}$ level.

Measurements of $B(E2)$, quadrupole moments, gyromagnetic ratios, and isomer shifts would provide important but indirect tests. The most direct test would be provided by the two-neutron–transfer amplitude discussed above. Another test has been suggested by Sheline[19]: the A dependence of the critical angular momentum, I_C. For this purpose, calculations (also, experiments) are needed for nuclei in different mass regions.

I am grateful to G. B. Hagemann for preprints and for discussions of her own and related experiments. I thank W. T. Pinkston and J. H. Hamilton for valuable comments.

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Asymmetries in Charged-Pion Photoproduction on Nucleons by 16-GeV Polarized Photons*

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Asymmetries in charged-pion photoproduction from hydrogen and deuterium have been measured with 16-GeV linearly polarized photons. Considerable energy dependence is seen in the natural-parity contribution to the π^-/π^+ ratio from deuterium, and in the unnatural-parity part of the cross section for $\gamma n \to \pi^- p$. The energy dependence of this latter cross section is consistent with the expected from a conventional pion Regge trajectory.

The use of linearly polarized photons to separate natural- and unnatural-parity exchanges in single-pion photoproduction has been discussed by several authors.[1] To leading order in t/s, photoproduction with photons polarized perpendicular (parallel) to the reaction plane proceeds by natural- (unnatural-) parity exchange in the t channel. The asymmetry

$$\Sigma = \frac{d\sigma_\perp/dt - d\sigma_\parallel/dt}{d\sigma_\perp/dt + d\sigma_\parallel/dt},$$

where $d\sigma_\perp/dt$ ($d\sigma_\parallel/dt$) denotes the cross section