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TITLE: A NUCLEAR STRUCTURE STUDY OF THE PROPOSED GAMMA-RAY LASER CANDIDATE NUCLEUS 186RE

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We present results of theoretical nuclear structure model calculations for the gamma-ray laser candidate nucleus 1^{66} Re proposed by Collins. Our calculations of this odd-odd transitional nucleus are based on an axially-asymmetric (particle plus triaxial rotor) model for constructing the orbitals of the odd nucleons that couple under the influence of the residual neutron-proton interaction. We include pairing correlations in the determination of these orbitals by using the BCS approximation with newly determined pairing strengths. The matrix elements of the residual neutron-proton interaction are obtained using phenomenological spin-dependent δ function potentials of both surface and volume forms. We examine the sensitivity of the calculated newroxitation level structure of 18^{6} Re to the strength of these potentials. Calculated energy levels of 18^{6} Re will be presented and compared with experiment. The impact of our results on the proposed use of 16^{6} Re as a gamma-ray laser will be discussed. In addition, based upon these and other model calculations to be described, we assess the level of effort necessary in a full-scale theoretical search for e visble candidate nucleus for a gamma-ray laser.

1. INTRODUCTION

The odd-odd transitional nucleus 186Re has an experimentally known isomeric state of spin and parity $J^{R} = 3^{+}$ at an excitation energy of approximately 150 keV. The state has a halflife T_{1/2} of 2 x 10⁵ years. Collins¹ has proposed ¹⁸⁶Re as a candidate nucleus for a gamma-ray laser on the basis of an as yet to be identified 7⁻ state lying close by the 8⁺ isomeric state. The 8⁺ storage level could be depopulated by El radiation to the 7⁻ transfer level, which would then cescede to the upper lasing level--the 3⁻ state at an excitation energy of 99 keV. The viability of the proposal of Collins rests upon the existence of ths 7⁻ state, its excitation energy relative to the 8⁺ storage state, and the strength of the El transition rate between these two states.

We report in this paper on our theoretical investigation of the low-lying level structure of 186Re with particular emphasis on the excitetion energies and nuclear structure properties of any 7° states near the known 8° isomeric state at approximately 150 keV. Our investigation consists of nuclear structure

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ABSTRACT

model calculations that are carried out in the following manner. We view the odd-odd transitional nucleus $75Re_{111}$ as the even-even core nucleus $74W_{110}$ plus an odd unpaired proton and an odd unpaired neutron that couple together under the influence of the attractive residual neutron-proton interaction. We obtain the orbitals (wave functions) of the unpaired proton by reproducing the low-lying level structure of $75Re_{110}$, viewing this nucleus as the $74W_{110}$ core plus a proton. Because $75Re_{110}$ is a transitional nucleus, we use an axiallyasymmetric model to calculate its low-lying level structure. Specifically, we use the particle plus triaxial-rotor model as formulated, for example, by Larsson, Leander, and Ragnarsson.² Similarly, to obtain the orbitals (wave functions) of the unpaired neutron, we use the same modal to reproduce the low-lying level structure of $74W_{111}$, viewing this nucleus as the $74W_{110}$ core plus a neutron. The calculations of these orbitals are destribed in detail in Sec. 2.

In Sec. 3, we calculate the matrix elements of the attractive residual ...eutron-proton interaction using the wave functions determined in Sec. 2. We consider two phenomenological spin-dependent δ function potentials to represent this interation. These are surface and volume δ function potentials whose strengths are determined by reproducing optimaily the known low-lying levels in 185Re. With this information, the remaining, unmeasured, low-lying levels of 166Re can be reliably predicted. We calculate the 185Re low-lying excitation spectrum in this way for both choices of the residual interaction, and compare our results with the aveilable experimental level information. Our conclusions from this work, expectations for future work, and assessment of the scope of s full-scale theoretical search for a viable candidate nucleus for a gemma-ray laser will be given in Sec. 4.

2. SINGLE-PARTICLE NAVE FUNCTIONS

Our starting point for the calculation of the two sets of single-particle wave functions that we require is the particle plus triaxialrotor model as formulated and coded by Larsson, Leander, and Ragnarsson.^{2,3} The particle-rotor Hamiltonian is derived from the meny-body Bohr-Hottelson Hamiltonian of an odd-mess system⁴ and is given by

$$H = \sum_{k=1}^{3} \frac{g^{2}}{2l_{k}} (J_{k} - j_{k})^{2} + H_{part} (\alpha) , \qquad (1)$$

where the I_k are the moments of inertia, and J_k and j_k are components of the total and single-particle angular momentum, respectively. The second term is the single-particle Hamiltonian in an adiabatic core field described by collective coordinates G. Equation (1) is actually obtained from the Bohr-Mottelson Hamiltonian by choosing the strong-coupling basis, which has the edvantage that the particle-rotation interaction then appears in the equation only in a Coriolis term,

Coriolis term =
$$-\sum_{k=1}^{1} \frac{g^2}{2l_k} (J_k \cdot j_k)^2 + H_{part}(\alpha)$$
, (1)

and a recoil term,

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recoil term =
$$\sum_{k=1}^{1} (\overline{n}^2 j_k^2 / 2I_k)$$
. (2)

The triaxial core assumption, appropriate to the transitional nuclei, is introduced to Eqs. (1)-(3) through a hydrodynamical model for the three moments of inertia, namely,

$$l_{\rm a} = (4/3) l_0 \sin^2 (\gamma + 2\pi k/3) , \qquad (4)$$

where γ measures the degree of sxial asymmetry or triaxiality and Ig is the moment of inertia associated with axial symmetry.

The single-particle Hamiltonian of Eq. (1), $H_{part}(G)$, required to calculate the single-particle wave functions X_{ν} , so that the diagonalization of Eq. (1) in the strong-coupling besis can occur, is constructed using the modified oscillator potential⁵

$$V_{esc} = (1/2)ha_0(\boldsymbol{e}_2, \boldsymbol{e}_4)\boldsymbol{\rho}^2 [1 \cdot (2/3)\boldsymbol{e}_3 \boldsymbol{P}_2(\cos \boldsymbol{\theta}_1)$$

+ $2\epsilon_{\theta}P_{\theta}(\cos\theta_{1})$]. (5)

This potential is expressed here in the stretched coordinate system⁵ for the case of quadrupole (z_2) and hexadecapole (z_4) deformations. In our actual celculations we include even higher deformation order, vir., z_6 . Two other ingredients of H_{part} necessary to fit accurately the level spectra of deformed nuclei are a spin-orbit term,

with coupling strength κ , and a quadratic orbital angular momentum term (to truncate the oscillator potential with increasing mass number A),

with coupling strength Kµ. With the total single-particle potential given by Eqs. (5)-(7), one obtains solutions of $H_{part}(\alpha)$ of the form

$$\chi_{v} = \sum_{\alpha,\Omega} C_{\alpha,\Omega}^{(v)} \psi_{\Omega}^{(q)} , \qquad (S)$$

with $\alpha = N, \hat{\ell}$, where N is the principal oscillator quantum number, $\hat{\ell}$ and j are the orbital and total angular momentum of the particle, and Ω is the projection of j along any one of the three principal axes. The basis wave functions $\Psi_{\Omega}^{(1)}$ are coupled harmonic oscillator wave functions referred to the stretched coordinate system.⁵ However, we wish to note that the entire formalism presented here can also be referred to the unstretched coordinate system in which no approximations are made in the coupling calculation. We have used the unstretched coordinate system in all of the calculations presented in this paper.

Finally, we account for the effects of pairing correlations by performing a standard BCS calculation on the adiabatic single-particle levels X_V . Therefore, the Fermi level and the pairing occupation factors are uniquely determined without additional adjustable parameters. In the BCS calculation, the pairing strengths $G_0 \pm G_1[(N-2)/A]$ are determined by reproducing the experimental pairing gaps Δ_n and Δ_p obtained from fourth-order mass difference equations.⁶

We now present our results in calculating the single-particle were functions χ_{ν} for the od:-proton nucleus ${}_{75}Re_{111}$ and the odd-neutron nucleus ${}_{74}W_{111}$. The final values of the input parameters for the two nuclei are presented in Table 1. In this table, the values of K and μ are taken from the extensive studies of Nilsson et al.⁵ and these were held fixed throughout. The values of the quadrupole (ϵ_2) and hexadecapole (ϵ_4) deformations were constrained to lie close to the transforms of the corresponding β_2 and β_4 values determined in the analysis of unclei. The value of ϵ_6 for 165 Re was taken from the systematic theoretical analysis of ground-state masses by Möller and Nim.⁷ The value of ϵ_6 for

 ^{185}W was taken to be zero for the present calculations. For 185_{Re} a value of $\gamma = 15.04^{\circ}$ was determined by adjustment to the measured excitation energy 646.0 keV of the bandhead of the K = $1/2 \gamma$ -vibrational band. A value of γ = 0.0° is used for 185W, as the only experimental evidence for a y-vibrational band in this nuceus is tentative, for a K = 3/2 y-vibrational band above 1 MeV in excitation. Since the presence of the odd nucleon in the 184W core polarizes this core somewhat, the excitation energy of the core 2* state, E(2*), is adjusted to reproduce the experimental ex-citation energy of the first-excited state in the odd-nucleon nucleus. The values of $E(2^*)$ in Table 1 should be compared to the true value of 0.1112 MeV. As already mentioned, the values of the pairing strengths G_0 and G_1 are adjusted to reproduce the experimental pairing gaps Δ_n and Δ_p . Finally, the parameters ξ_{pair} and ξ_{Coriolis} are attenuations on the pairing factor (exponential) and the Coriolis term (multiplicative), which are normally of unit value. However, it is well known that attenuation of these two terms can sometimes improve agreement with experiment in axially-symmetric cases. We have found that a value of $\xi_{\text{Coriolis}} = 0.9$ for ¹⁸⁵W (axially symmetric in our present treatment) gives better agreement with the experimental level spectrum than does the unit value.

The levels (and therefore the corresponding wave functions) calculated using the parameters contained in Table 1 are compared with the experimental levels in Tables 2 and 3. In Table 2 we compare calculated and experimental levels for the first three evenparity bands of 1^{85} he. The quite good agreement indicates that the corresponding wave functions can be used with confidence in calculating the residual n-p interaction matrix elements for 1^{86} Re, to be discussed in Sec. 3. We reach a similar conclusion with Table 3, in which we compare calculated and experimental levels for the first three odd-perity bands of 1^{85} Ne. Here, the agreement batween calculation and experiment is not as good overall as for 1^{85} Re. However, the errors in the 1^{85} Ne wave functions that are required in predicting the locations of any 7⁻ states in 1^{85} Re are quite small. We now turn to a discussion of the calculations of the residual n-p interaction matrix elements using the single-particle wave functions that have been described here. . .

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Parameter	Odd-Proton Nucleus	Odd-Neutron Nucleus 0.0636	
ĸ	C.0 62		
μ	0.614	0.393	
e2	0.230	0.240	
E4	0.130	0.068	
٤6	-0.013	0.0	
γ (deg)	15.04	0.0	
E(2 ⁺) (MeV) G ₀ ·(MeV) G ₁ (MeV)	0.1187 20.435 7.4	0.1200 20.150 7.4	
Δp (MeV)	0.826		
Δn (MeV)	~~	0.783	
5peir	1.0	1.0	
Coriolis	1.0	0.9	

Table 2. Comparison of Calculated and Experimental Low-Lying Even-Parity Bands of the Odd-Proton Nucleus ¹⁸⁵₇₅Re₁₁₀

Band		Calcuated <u>(keV)</u>	Experimental (<u>keV)</u>
<u>5</u> [402]	5/2+	0.0	0.0
	7/2+	125.1	125.348
	9/2+	284.5	284.1
	11/2+	476.8	475.6
	13.2+	699.0	697.0
	15/2+	950.5	949.5
	17/2+	1227.2	1230.0
K=+ y-vib.	1/2+	646.0	646.11
K =<u>1</u> γ ·vib. (<u>\$</u> [402])	3/2+	708.5	717.42
	5/2+	786.9	767.3
$\frac{1}{2}$ [411]	3/2+	869.5	874.81
	1/2+	888.9	880.27

Table 3 Comparison of Calculated and Experimental Low-Lying Odd-Parity Bands of the Odd-Neutron Nucleus $^{185}_{-74}W_{111}$

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Band		Calcuated (keV)	Experimental (<u>keV)</u>
3 <u>2</u> [512]	3/2-	0.0	0.0
	5/2:	64.4	65.86
	7/2	204.1	173.68
	9/2	313.9	302.0
	11/2	564.9	480.0
1/2 [510].	1/2+	8.9	23.54
	3/2+	87.6	93.30
	5/2+	195.1	187.88
	7/2.	343.5	338.0
	9/2-	544.3	490.0
	11/2	745.5	706.0
7 [5 03]	7/2.	246.8	243.5
	9/2-	419.5	390.8
	11/2-	630.4	570.0

3. RESIDUAL NEUTRON-PROTON INTERACTION AND THE 186RE SPECTRUM

The simplest generalization of Eq. (1) for two nucleons is

$$H = \sum_{k=1}^{2} \frac{u^{2}}{2I_{k}} (I \cdot j_{n} \cdot j_{p})_{k}^{2} + H_{pp} + V_{np} , \qquad (9)$$

where the rotational and single particle terms of H have the same significance as in Eq. (1), and V_{np} in the residual neutron-proton interaction. Historically, only the axially-symmetric case was considered⁹,9¹⁰. This was in part due to a lack of detailed experimental information in odd-odd nuclei, a lack of the requisite computational abilities, and to a realization that the differences due to assumed axial asymmetries were offset by the uncertainties in V_{np} .

However, each of these difficulties has been, or is currently being overcome. With the advent of new heavy ion accelerators and 4% detectors, prodigious amounts of data are becoming available. Larger computers allow more basis states--an essential point since relaxing the requirement of axial symmetry results in Hamiltonian matrices an order of magnitude larger than for the case of axially symmetric systems. Finally, the increased computing power also allows the calculation of the neutron-proton interaction from potentials based on nucleon-nucleon scattering. Further, considerable work on the magnitude of Vnp has been done by R. Hoff and his collaborators¹¹. In this paper we shall calculate V_{np} from simple phenomenological interactions such as a delta function potential. Our choice for the delta function includes both a spin-independent as well as a spin-dependent part. Our selection follows closely the work of Sood et al.12,13, although in addition to a purely central delta interaction, we also allow a tensor interaction with no radial dependence to contribute.

It is relevant to briefly discuss the case of axial symmetry, since the systematics of the matrix elements of the neutron-proton interaction is similar for the two instances. If Ω_p and Ω_n are the projections of the proton and neutron single-particle angular momenta along the symmetry axis, then $\kappa=\Omega_p$ + Ω_n where K is the projection of the angular momentum of the core along the axis. It was demonstrated by Gallagher and Moszkowski⁸ that if the projection of each of the single nucleon's spin is aligned or anti-aligned, the matrix element of V_{np} is attractive. If one is aligned with the direction of the projection of the orbital angular momentum and the other is anti-aligned, then the matrix element is repulsi.e.

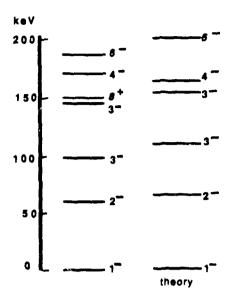
A simple representation of V_{np} is

$$\langle \mathbf{I} \mathbf{K} | \mathbf{V}_{np} | \mathbf{I} \mathbf{K} \rangle = \mathbf{A} + (\cdot)^{\mathsf{t}} \delta_{\mathbf{k},0} \mathbf{B}$$
(10)

The first term is usually referred to as a Gallagher-Moszkowski matrix element. The second term is the so-called Newby term⁹. The magnitudes of A and B are typically a few hundreds and tens of keV, respectively. In our work, the matrix element is explicitly calculated.

From the single particle wave functions and energies calculated, as described in Sec. 2, and with the matrix elements of V_{np} calculated as described above, one may calculate the structure of 186Re. Our results for the negative parity states are shown in Fig. 1. We omit here a discussion of the positive parity states, since we are primarily interested in the possibility of a low-lying 7⁻ level. In fact, there are several 7⁻ levels; one is a dominant member of the ground-state band; others may be formed from other bands. The physical levels are, of course, mixtures of the simple states thus formed. The lowest 7⁻ lies above 300 keV and therefore 186Re can uniortunately be eliminated from consideration as a candidate for a gamma ray laser.

This points out two important facts: nuclear structure calculations can be useful as a guide to whether a particular nucleus may be a possible candidate. It also reaffirms that it is easier to eliminate a nucleus than to demonstrate that a given nucleus meets the necessary criteria.



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Fig. 1. The low lying negative parity states of 186_{Re} calculated as described in the text. The interaction used in the calculation has not been optimized.

4. DISCUSSION AND CONCLUSION

We have demonstrated in this paper that it is possible to eliminate ¹⁸⁶Re from consideration as a candidate for a gamma-ray laser. Similar techniques may be applied to other nuclei to test their applicability. However, this only addresses one aspect of the problem--that of eliminating candidates. The other aspect, namely, that of actually proposing promising possibilities, is more difficult. In order to do this, several refinements to our model currently under way will have to be completed.

The neutron-proton interaction V_{np} was calculated above from a simple central delta interaction. However, it is known that the true interaction contains appreciable non-central components. These are currently being calculated using G-matrix techniques pioneered by Kuo and Brown.

A further refinement applies both to the odd-A and odd-odd cases. In the above discussion the pairing interaction was included in an *ad hoc* manner, which leads to uncertainty. For example, should 185_{Re} be considered as a particle outside a 184_{Re} core or a hole in 186_{Re} ? If the mass 184 and 186 nuclei do not differ appreciably, it 13

probably irrelevant from a practical point of view, although the ambiguity is still unseemly. Both of these objections may be overcome by using the results of Dönau and Frauendorf¹⁴, which are based on earlier work by Kerman and Klein¹². In this case the Hamiltonian takes the form of an array:

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$$H = \begin{pmatrix} E_{R} + \Gamma + \lambda & \Delta \\ & & \\ & & \\ & & \\ & & \\ & & \Delta & E_{R} - \Gamma - \lambda \end{pmatrix}$$
(11)

The basis states are the core states of A+1 and A-1. Since the energies of these core states enters explicitly, they may have very different properties. Further, these even-even core states may be calculated explicitly. Ideally they would be calculated by self-consistent, multi-configurational Hartree-Fock. Such an approach would be more basic, but prohibitively expensive if one wishes to Fock. Such an approach would be more basic, but prohibitively expensive if one wishes to explore many nuclei. We choose to obtain the core states by numerically solving the Bohr Hamiltonian using a variant of the techniques pioneered by Hess et al^{16} . This is somewhat similar to recent work by Bennour et $al.^{17}$ The analog of eq. (1) has been derived for the case of two nucleons outside a core. Work in these directions is continuing.

REFERENCES

 C. B. Collins, "Coherent and Incoher-ent Upconversion Techniques for the Pumping of a Gamma-Ray Laser," Proceed. IST/IDA Gamma-Ray Laser Workshop, Washington D.C., May 21-22, 1985, Eds., B. Balko, L. Cohen, and F. X. Hartman, Inst. for Defense Analysis report M-162, January 1986, p. 137.
S. E. Larsson, G. Leander, and I. Ragnarsson, "Nuclear Core-Quasiparticle Cou-pling," Nucl. Phys. A 307, 189 (1978).
We wish to thank G. Leander for kindly providing us with copies of his source codes for the particle plus triaxial-rotor model.
A. Bohr and B R. Mottelson, 1. C. B. Collins, "Coherent and Incoher-

4. A. Bohr and B R. Mottelson, "Collective and Individual-Particle Aspects of

"Collective and Individual-Particle Aspects of Nuclear Structure," Mat. Fys. Medd. Dan. Vid. Selsk. 27.No. 16 (1953). 5. S. G. Nilsson et al., "On the Nuclear Structu. and Stability of Heavy and Superheavy Elements," Nucl. Phys. A131, 1 (1969). 6. D. G. Madland and J. R. Nix, "New Model of the Average Neutron and Proton Pairing Gaps," Nucl. Phys. A476, 1 (1988). 7. P. Möller and J. R. Nix, "Nuclear Masses from a Unified Macroscopic-Microscopic Model " At. Data Nucl. Lata Tables (in press).

Masses from a Unified Macroscopic-Microscopic Model," At. Data Nucl. Data Tables (in press). 8. C. J. Gallagher and S. A. Moszkowski, "Coupling of Angular Momentum in Odd-Odd Nuclei," Phys. Rev. 111, 1282 (1958). 9. N. D. Newby, Jr., "Selection Rules in the Odd-Even Shift of Certain Nuclear Rotation Bands," Phys. Rev. 124, 2063 (1962).

10. J. P. Boisson, R. Piepenbring and W. Ogle, "The Effective Neutron-Proton Interaction in Rare-Earth Nuclei," Phys. Rept. 26, 99 (1976). 11. R. W. Hoff et al., Nucl. Phys. A 437,

٠

26, 99 (1976). 11. R. W. Hoff et al., Nucl. Phys. A 437, 285 (1955). 12. P. C. Sood and R. N. Singh, "Energy Levels in 238Np and 240,242,244Am Based on Residual Interaction Studies," Nucl. Phys. A 373, 519 (1982). 13. P. C. Sood, "Low-Lying Two-Particle States in the Nucleus 236Np," Z. Phys. A 318, 111 (1984). 14. F. Dönau and S. Frauendorf, "Description of Odd Transitional Nuclei in Terms of Core-Quasi-Particle Models," Phys. Lett. 71B, 263 (1977). 15. A. Riein, "Algebraic Methods for a Direct Calculus of Observables in the Theory of Nuclear Band Structure," Adv. in Nucl. and Part. Phys. 4, 39 (1981). 16. P. Hess. M. Seiwert, J. Maruhn and W. Greiner, "General Collective Model and its Application to 238U", Z. Phys. A 296, 147 (1980).

Application to 2000, 2. Phys. & 296, 147 (1980). 17. L. Bennour, J. Libert, M. Meyer and P. Quentin, "A Self-Consistent Description of the Spectroscopic Properties of Odd-Odd Nuclei," Nucl. Phys. A 465, 35 (1987).