

THE PARTICLE + TRIAXIAL ROTOR MODEL: A USER'S GUIDE

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Introduction

This manual is a supplementary guide for the particle + triaxial rotor computer codes presented at the Risö Hands-On Nuclear Structure Theory Workshop in June, 1992 and contains only a few minor changes from the Oak Ridge (August, 1991) version. It is written with the intention that the novice will be able to get started using these codes intelligently with this manual and little otherwise direct guidance. For each of the codes described here, an extensive set of comments and description of the input data can be found at the very beginning of the program. These comments are reprinted here and form the bulk of this manual. Additional information concerning how these programs work, the physical meaning of the model parameters and suggestions for finding reasonable initial values are provided here, along with sample input files and some references. After a little experience using these codes and interpreting their results, it is hoped that the erstwhile novice will find that the comments written into the codes are sufficiently detailed and complete that this manual quickly becomes unnecessary.

General features of the computer codes

Two different sets of particle-rotor codes are described here. The first begins with a Woods-Saxon parameterization of the deformed mean field, while the second uses a Modified Oscillator potential. In each case the calculations proceed as follows:

1. At a fixed deformation (selected by the user), the Schrödinger equation describing the single-particle motion in the deformed field is solved, creating a set of single-particle energies and eigenfunctions (Nilsson states). The user must specify whether the calculation is to be done for proton or neutron orbitals (not both) according to the identity of the odd particle.
2. From the Nilsson states generated in step 1, the user selects a set from which the particle + rotor strong coupling basis states will be constructed. Within this set of Nilsson orbitals, all the single particle matrix elements needed for the particle + rotor Hamiltonian and the M1/E2 calculations are computed, including $\langle j_+ \rangle$, $\langle j_z \rangle$, $\langle s_+ \rangle$, etc. Typically, selecting 5 such states above and below the Fermi level is sufficient to ensure numerical convergence, but as many as 15 can be retained. Note that these codes treat even multipoles only in the deformed field (i.e., no octupole deformation), so there is no mixing between positive and negative parity orbitals. Thus, the user must specify the parity of the orbitals to be retained for later use. There is no restriction to unique parity states (high j-shells) in these codes.
3. From the single particle energies computed in step 2, the residual pairing interaction is treated within the BCS approximation. This implies that for each deformed single-particle state, the quasiparticle energy and the pairing factors u and v are computed, from the single-particle energies, the Fermi level λ and the pairing gap Δ . If this calculation is made by adopting a standard value for the pairing strength parameter G , then the Fermi level and the pairing gap are derived quantities, and not input parameters. The blocking effect is roughly included by requiring that λ correspond to the odd number of particles, Z or N . (Alternatively, λ and Δ can be input directly.) Next, using the Nilsson states selected in step 2 (or some subset of these), the particle + triaxial rotor

Hamiltonian matrix is constructed and diagonalized for a selected range of values for the total spin I , in the 1-quasiparticle strong coupling basis. The user must provide some information about the core energy spectrum (moments of inertia), for example, by specifying the energy of the first 2^+ state in the effective even-even core. Various angular momentum expectation values (e.g., $\langle I \cdot j \rangle / |I|$) are calculated from the energy eigenvectors.

4. Electromagnetic matrix elements, both diagonal and off-diagonal, are calculated from the eigenvectors of the particle + rotor Hamiltonian generated in step 3. The diagonal matrix elements are displayed as the static moments (electric quadrupole moment Q_s , and the magnetic dipole moment μ), in units of e-barn and nuclear magnetons (μ_N), respectively. Note that the electric quadrupole moment is the spectroscopic moment, which is directly observable in experiments, and not just the intrinsic moment Q_0 . The off-diagonal matrix elements are displayed as $B(E2)$'s and $B(M1)$'s (in $(eb)^2$, and $(\mu_N)^2$, respectively), and as γ -ray partial transition rates, $T(E2)$ and $T(M1)$. Furthermore, for mixed $E2/M1$ transitions, the mixing ratio $\delta(E2/M1)$ is computed. All the transition rate calculations use the computed γ -ray energies when needed.

For the Woods-Saxon version of the particle + rotor package of computer codes, the following programs perform the steps outlined above:

Step 1: SWGAMMA
 Step 2: WSDCUP
 Step 3: ASYRWS
 Step 4: PROBAWS

The first program, SWGAMMA, is the same program also described at this workshop for cranking applications. A sufficiently detailed description of SWGAMMA is given here so that this discussion remains self-contained, but the reader is reminded that additional notes have been prepared and distributed at this workshop by Ramon Wyss.

For the Modified Oscillator version of this model, the following programs perform the steps described above:

Step 1 and Step 2: GAMPN
 Step 3: ASYRMO
 Step 4: PROBAMO

Since these two packages of codes are only different implementations of the same basic model, many strong similarities necessarily exist between the versions, and the structures of the ASYR and PROBA programs are particularly close. Even so, some important differences remain, mainly due to the different choices made in SWGAMMA and GAMPN for the basis states of the single-particle orbitals. A more detailed description is given below for each of these programs, and their similarities and differences should become quite clear. In either version, however, the most important parameters that must be assigned by the user are the deformation coordinates and the core energy spectrum (i.e., moments of inertia). Since the general considerations for determining reasonable values for these parameters are the same for either the Woods-Saxon or the Modified Oscillator version, some guidelines and suggestions are now given, followed by some general

comments about Coriolis attenuation and the recoil terms.

Selecting the deformation parameters and core moments of inertia

Clearly, the choice of the shape parameters is crucial in this model, and they must be chosen carefully and with clear justification. Generally, these could be taken either from experiment or theory, and in some cases can be extracted from a TRS database. Also, a number of tabulations exist in the literature that either give deformation parameters directly, or the intrinsic quadrupole moment or some related quantity (especially for even-even nuclei). Among the well-known tabulations are:

P. Möller and J. R. Nix, Atomic Data and Nuclear Data Tables 26 (1981) 165. This reference includes computed masses and intrinsic moments Q_0 for over 4000 nuclei. These are computed with the folded-Yukawa potential.

R. Bengtsson et al., ADNDT 35 (1986) 15, which gives predicted ground state deformations for even-even nuclei from Sm to Pt in terms of the Modified Oscillator potential (ϵ_2 , ϵ_4 parameters).

W. Nazarewicz et al. Nucl. Phys. A512 (1990) 61, which gives predicted bandhead deformations for odd-proton rare-earth nuclei (Eu - Au) in the Woods-Saxon potential. For some nuclei, significantly different deformations are expected for certain configurations (shape coexistence).

S. Raman et al., ADNDT 36 (1987) 1, which is a compilation of 2^+ energies of even-even nuclei and intrinsic quadrupole moments Q_0 derived from a variety of experimental measurements.

Thus, obtaining estimates for the deformation parameters may require converting between the ϵ and β parameterizations and/or deriving them from Q_0 . For axially symmetric deformations that are not too large (i.e., $-0.2 \leq \beta_2 \leq 0.4$, and $-0.05 \leq \beta_4 \leq 0.15$, or so), the necessary relations are

$$\epsilon_2 \sim 0.944 \beta_2 - 0.122 \beta_2^2 + 0.154 \beta_2 \beta_4 - 0.199 \beta_4^2$$

$$\epsilon_4 \sim -0.852 \beta_4 + 0.141 \beta_4^2 + 0.122 \beta_2 \beta_4 + 0.295 \beta_2^2$$

$$Q_0 \sim \frac{4}{5} Z R_0^2 \epsilon_2 \left(1 + \frac{1}{2} \epsilon_2\right)$$

and

$$Q_0 \sim \frac{3}{\sqrt{5}\pi} Z R_0^2 \beta_2 (1 + 0.36 \beta_2)$$

In the expressions for Q_0 , the contributions from the hexadecapole terms (ϵ_4 and β_4) have been ignored. Further discussion of these points can be found in R. Bengtsson et al., *Physica Scripta* 39 (1989), 196, and R. W. Hasse and W. D. Myers, *Geometrical Relationships of Macroscopic Nuclear Physics* (Springer Verlag, 1988).

Excluding well-deformed axially symmetric rotors, the predicted values for the gamma deformation are more problematic, and are usually not appropriate for a particle-rotor analysis. For example, the gamma deformation predicted from TRS calculations in general cannot be expected to be directly applicable to the particle + rotor model, because of the very different treatments of the collective rotations (even when γ lies within the "collective sector" of the cranking model). Nonetheless, when significant triaxiality or γ -softness is expected from TRS maps, the particle-rotor user should be particularly careful to look for distinctive features in the experimental data that may signal the importance of the γ degree of freedom. Such distinctive features may include signature splitting in energies and B_{M1}/BE₂ ratios, "anomalous" static bandhead moments, unexpected yrare bands or low spin states, etc. In those cases where the neighboring even-even nuclei are reasonably well known and the quasi-gamma band appears at low energy, the triaxiality parameter can be estimated from the rigid triaxial rotor model. If the ratio of the core 2^+ energies is denoted by X , this gives

$$\gamma = \frac{1}{3} \arcsin \sqrt{\frac{9}{8} \left[1 - \left(\frac{X-1}{X+1} \right)^2 \right]}, \quad X = \frac{E(2_2^+)}{E(2_1^+)}$$

However, recall that the spectrum of an even-even triaxial rotor is symmetric about $\gamma=30^\circ$, i.e., a "prolatish" rotor with $\gamma=+20^\circ$ and an "oblatish" rotor with $\gamma=+40^\circ$ have the same energy spectrum, and thus the ratio of 2^+ energies alone cannot distinguish between the two alternatives. The E₂ properties are very different though, and the energy spectra as well as E₂ properties in the odd-A nucleus are usually strikingly different. Thus, γ can be estimated from the energy spectrum of the neighboring even-even nucleus, but generally it is ultimately treated as a parameter to be fitted to the properties of the odd-A nucleus. Frequently, the properties of the odd-A nucleus depend very sensitively on the gamma deformation.

The second crucial parameter that the user must supply is the energy of the 2_1^+ state in the effective core. For the triaxial case, the 3 moments of inertia are assumed to be related by a hydrodynamical expression, and thus an overall moment of inertia parameter is determined by the energy of the 2_1^+ core state. Of course, this energy is strongly coupled to the assumed deformation (and also to the proton and neutron pairing gaps). In those applications where the deformation is supposed to reflect the observable properties of a neighboring even-even nucleus, the physical 2_1^+ energy can be used to estimate the core moments of inertia. However, this generally underestimates the effective core moments of inertia. One reason why this estimate can only be rough is because the physical even-even nucleus almost never obeys the rigid rotor energy law very well above spin 6 or so. Instead, a gradual increase in the moment of inertia is almost always observed and thus results in a varying moment of inertia. If the ground band of an even-even rotor must be approximated with a fixed moment of inertia (rigid core approximation), then the effective core 2_1^+ energy must be

less than the energy of the physical core state, typically about 15% less. A convenient compilation of experimental energies in even-even nuclei can be found in M. Sakai, ADNDT 31 (1984) 399.

The core 2_1^+ energy can also be estimated from the deformation, and a rough estimate is provided by Grodzins' relation:

$$E(2_1^+) \approx \frac{1225}{\beta^2 A^{\frac{7}{3}}} \text{ (MeV)}$$

(To the accuracy of this estimate, β and ϵ probably should be used interchangeably.) This estimate can be selected in either version of the ASYR program. More sophisticated estimates can be found elsewhere (e.g., in R. Bengtsson and S. Åberg, Phys. Lett. 172B (1986) 277, and in the accompanying lecture notes) but are not pursued here.

Comments on the recoil terms and Coriolis attenuation

The recoil terms are quadratic operators like j_+^2 that occur in the particle + rotor model, and some debate remains over whether these should be treated as one-body or two-body operators. If they are treated as two-body operators, then their matrix elements are derived by inserting a complete set of intermediate states (including 3-quasiparticle as well as 1-qp states) and summing appropriately, as given in E. Osnes et al., Nucl. Phys. A253 (1975) 45. If they are treated as one-body operators, then the single-particle matrix elements are multiplied by the same $(uu' + vv')$ pairing factors as for the Coriolis terms. An explicit discussion of this point, and some justification for the latter method is presented in L. Bennour et al., Nucl. Phys. A465 (1987) 35. These two procedures are not equivalent when pairing is included, and which method is "correct" seems to be as much a matter of philosophy as physics (at least as long as the simple BCS treatment of pairing is used). In the present programs, both options are available, but the two-body treatment requires extra computation in WSDCUP or GAMPN. Also, a small, constant "core contribution" that arises in the two-body treatment has been neglected here, and this makes the calculation of the angular momentum expectation values (tabulated for the particle-rotor energy eigenvectors) approximate. This neglect does not affect the excitation energies at all. Finally, current experience with these codes has found similar results with either of these two options, and so the simpler one-body treatment is recommended.

The most famous difficulty with the particle + rotor model is that the Coriolis coupling between Nilsson states often seems too large, especially for unique parity orbitals. The exact reason for this is still not clear, although many possible causes have been proposed. (However, it must be recognized that in a particular calculation, there are many many possible remedies within the model that may or may not be physically justified. For example, shifting the Fermi level or changing the deformation will certainly influence the mixing between Nilsson states.) Two "ad hoc" approaches exist that are commonly employed when such difficulties arise and cannot be overcome by "reasonable means". Both approaches introduce an additional parameter that has little clear justification other than to reduce the coupling between the Nilsson states. One approach is to multiply all off-diagonal matrix elements by an "attenuation factor" $\chi_{si}(\zeta)$, while the other raises the $(uu' + vv')$ pairing factor to some power η .

Thus, $\zeta=1.0$ and $\eta=1.0$ correspond to no attenuation of these matrix elements. Both options are available in these codes, and both should be avoided if at all possible. In those cases when an attenuation seems justified, $\zeta \approx 0.7$ and $\eta \approx 5$ have been commonly used.

The comments built into each computer code are given next, along with sample input files and a few additional remarks.

The Woods-Saxon programs:

```
C
C
C   PROGRAM SWGAMMA
C
C
C   NAMELIST
*       /DYNAMIC/ BETA2,BETA4,GAMM,ECUTB,IZ,IN,NMAXP,NMAXN,IZNAK,
*               IENDD
*       /INTDAT/  NPRINT,IPRINT,LCOUNT,JSIGN,IPLLOT,LAMCUT,NAZWIS,
*               IDYSK,NMAXN,IZNAK,IDIM,IAUTO,ILGAUS,IFONLY,NET
C
C
C   NPRINT   -   THE NUMBER OF THE MATRIX ELEMENTS IN AUXILIARY
C               PRINT (PREFERABLY 0, HUE,HUE).
C
C   IPRINT   -   THE NUMBER OF LINE PRINTOUT FOR SINGLE PARTICLE
C               SPECTRUM (FOUR LEVELS PER ONE LINE).
C
C   IDYSK     -   IF (IDYSK.EQ.0) OUTPUT ON THE MAGNETIC TAPE
C               IF (IDYSK.NE.0) OUTPUT ON THE PERMANENT FILE
C
C   IPLLOT    -   IF (IPLLOT.EQ.0) ILLUSTRATIVE PLOTS ARE NOT
C               PRINTED.
C
C   JSIGN     -   IF (NE.(-9)) WRITE OUTPUT (S.P. ENERGIES AND
C               WAVE FUNCTIONS) ON TAPE NW (-10)
C               IF JSIGN=-8 WAVE FUNCTIONS ARE NOT RECORDED
C
C   LCOUNT    -   THE NUMBER OF THE ACTUAL SET OF DATA (INCREASED
C               BY 2 AT A GIVEN DEFORMATION)
C
C   ILGAUS    -   THE NUMBER OF POINTS IN THE NUMERICAL INTEGRATION
C               OVER FI (MAX. = 40)
C
C   LAMCUT    -   THE MAXIMUM DIFFERENCE BETWEEN LAMBDA AND LAMBDA1
C               IN THE INTEGRATION OF THE MATRIX ELEMENTS
C               (MAXIMUM = 2*NMAX+1)
C
C   IFONLY    -   IF .EQ.0  BOTH NEUTRONS AND PROTONS
C               IF .EQ.1  NEUTRONS ONLY
C               IF .EQ.2  PROTONS  ONLY
C               IF .EQ.3  AUXILIARY PLOTS ONLY
C
C   ECUTB     -   PARAMETER OF THE BASIS CUT OFF (IN MEV).
C               REASONABLE CHOICE IS 100. TO 150. BUT IT MUST
C               BE CAREFULLY TESTED BEFORE CALCULATION.
C
C               IN THIS VERSION ECUTB WILL BE TAKEN AS A STARTING
C               VALUE MODIFIED IN SUCH A WAY THAT THE TOTAL
C               NUMBER OF BASIS STATES IS AS CLOSE TO IDIM AS
```


C POSSIBLE.
 C
 C IDIM - THE NUMBER OF LOWEST LYING BASIS STATES
 C
 C INPUT DATA SECOND RECORD
 C
 C NAZWIS - IF (NAZWIS.EQ.0) WAHLBORN PARAMETERS,
 C IF (NAZWIS.EQ.1) ROST PARAMETERS,
 C IF (NAZWIS.EQ.2) CHEPURNOV PARAMETERS,
 C IF (NAZWIS.EQ.3) OPTIMIZED PARAMETERS,
 C IF (NAZWIS.EQ.4) UNIVERSAL PARAMETERS *& - Default.*
 C IF (NAZWIS.EQ.5) PARAMETERS READ IN THE FORMAT
 C
 C FORMAT(7(F7.4,3X))
 C
 C THE PARAMETERS READ ARE VO,XAPPA,XLAM,ROC,ROSO,AOC,AOSO
 C
 C NMAXP - MAXIMUM NUMBER OF THE HARMONIC OSCILLATOR SHELLS
 C (FOR PROTONS),
 C
 C NMAXN - MAXIMUM NUMBER OF THE HARMONIC OSCILLATOR SHELLS
 C (FOR NEUTRONS).
 C
 C ILS - (N-N1).LT.ILS MATRIX ELEMENTS ARE RETAINED.
 C (FOR NEUTRONS).
 C
 C IZ - PROTON NUMBER A=IZ+IN
 C
 C IN - NEUTRON NUMBER A=IZ+IN
 C
 C FACC - $HOMO = FACC * 41. / A^{(1./3.)}$.
 C
 C IZNAK - IZNAK.EQ.(0,1,2) - THREE KINDS OF BETA4
 C PARAMETRISATION
 C
 C IENDD - IF (IEND.NE.0) STOP "END OF INPUT DATA"
 C
 C IAUTO - IF (IAUTO.EQ.1) IZ DETERMINES NMAX AND IDDIM
 C AUTOMATICALLY
 C
 C NET - IF .EQ.0 DEFORMATIONS DEFINED BY THE READ STMT.
 C IF .GT.0 THE NET-TH ROW OF THE DEFORMATIONS
 C PREPARED BY THE LDPMIN-PROGRAM WILL
 C BE USED
 C IF .LT.0 THE 'RECTANGULAR' DEFORMATIONS DEFINED
 C AS $X = BETA2 * \cos(30 + GAMMA)$ AND
 C $Y = BETA2 * \sin(30 + GAMMA)$ ARE DEFINED BY
 C THE READ STMT. (X := BETA2, Y := GAMMA)
 C ATTENTION: ONE HAS TO DEFINE X AND Y
 C FOR EACH MESH-POINT SEPARATELY (I.E.

C YOU CANNOT TAKE ADVANTAGE OF NO
C REPEATING PREVIOUSLY DEFINED VARIABLE
C WHEN NAMELIST IS USED).
C
C

Now a few notes relevant for the particle + rotor user:
Note that the input parameters are read through a NAMELIST directed READ statement, and furthermore that most of the parameters are automatically set to standard values which do not need to be changed. At minimum, the user must specify the proton and neutron numbers of the nucleus of interest (IZ and IN) the deformation coordinates, (BETA2, GAMM and BETA4), and whether the calculation is to be made for protons or neutrons (IFONLY = 2 or 1, respectively). For the particle + rotor applications, only the proton or the neutron calculations should be made here, and not both. Also, certain technical parameters must be selected that control the number of basis states and the maximum oscillator number N. Standard values for these can (and should) be chosen by setting IAUTO=1. More than one calculation can be done with the same input file (e.g., more than one deformation), by setting IENDD=0 in the DYNAMC list, and then repeating this card for each desired deformation. Then for the last calculation, set IENDD=1.

** Important restriction: Note that for particle + rotor applications, only one 60° sector in the (β , γ) plane is distinct (the others simply correspond to permutations of the labels on the nuclear axes). However, SWGAMMA treats the intrinsic x-axis as the quantization axis, while the particle + rotor codes use the intrinsic z-axis. In order to match the requirements of these different codes, only one particular 60° sector can be used in SWGAMMA for later particle + rotor applications. In particular, the shape parameters must be chosen so that

BETA2 > 0 (always)
GAMM = -120. for axially symmetric prolate shapes
-120. < GAMM < -90. for "prolatish" triaxial shapes
+30. ≤ GAMM < +60. for "oblatish" triaxial shapes
GAMM = +60. for axially symmetric oblate shapes.

Note that GAMM = -90. is NOT ALLOWED, and is not equivalent to GAMM = +30.

A sample input file (named, e.g., IR179SWG.DAT) that could be appropriate for prolate states in ¹⁷⁹Ir is:

```
$INTDAT IFONLY=2 IAUTO=1 $END
$DYNAMC BETA2=0.26, BETA4=-0.004, GAMM=-120., IZ=77, IN=102 $END
```

INPUT FILE FOR SWGAMMA, FOR 179Ir

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C**** PROGRAM WSDCUP
C
C   VERSION: JULY, 1991
C
C   DISTRIBUTED AT THE OAK RIDGE THEORY WORKSHOP, AUG 1991, FOR USE
C   WITH OTHER WOODS-SAXON CODES SWGAMMA (WHICH CALCULATES THE
C   DEFORMED SINGLE PARTICLE ORBITALS [EIGENVALUES AND EIGENVECTORS]
C   AND PRECEDES WSDCUP), ASYRWS (DIAGONALIZES THE PARTICLE + ROTOR
C   HAMILTONIAN) AND PROBAWS (CALCULATES M1/E2 MATRIX ELEMENTS FROM
C   THE PARTICLE + ROTOR EIGENVECTORS)
C
C
C   WSDCUP CALCULATES GENERALIZED DECOUPLING FACTORS FOR TRIAXIAL
C   ROTOR + PARTICLE MODEL (NUCL. PHYS. A307 (1978) 189) IN THE BASIS
C   /N NZ LAMBDA SIGMA>. PHASES AS IN FUNNY HILLS WOODS-SAXON, OR
C   FOLDED YUKAWA OF NIX ET AL. GENERATES OUTPUT FILE 17 FOR USE BY
C   PROGRAM ASYRWS.
C
C   THE MATRIX ELEMENTS ARE FROM THE TABLE OF BOISSON AND PIEPENBRING
C   [NUCL PHYS A168 (1971) 385] OF L+ 9DENOTED RP) L- (RM) AND S+ (SP).
C   S- IS OBTAINED BY REVERSING THE SIGN OF THE ARGUMENTS IS.
C   L= (RM) SIMILARLY REQUIRES REVERSED SIGN OF THE ARGUMENT L.
C   ASYR CONJ /N NZ LAM SIG> = (-1)**(N-1/2-SIG) /N NZ -LAM -SIG>.
C   NOTE THAT BOISSON AND P. FORGET SIGN CHANGE FOR NEGATIVE LAM.
C
C**** THE ORIGINAL VERSION CODED IN LUND IN AUGUST, 1983, BY GEORG A.
C   LEANDER, OAK RIDGE.
C**** THIS IS A VERSION FOR VAX BY LEANDER, OAK RIDGE, DECEMBER, 1983.
C   INPUT UNIT (FILE3) SHOULD BE THE OUTPUT FILE FROM THE WOODS-SAXON
C   CODE OF DUDEK AND NAZAREWICZ.
C   THE BASIS STATES OF THAT CODE COME IN BLOCKS WITH OMEGA=1/2,
C   -3/2, 5/2, -7/2, ... AS ASSUMED BELOW, PROVIDED THAT GAMMA IS IN
C   THE INTERVAL -120 .LE. GAMMA .LT. -90 OR +30 .LE. GAMMA .LE. 60.
C
C ** NOTE THAT GAMMA = -90 IS IMPROPER, AND GIVES INCORRECT RESULTS! **
C
C   FURTHERMORE, THE WOODS-SAXON INPUT SHOULD BE IFONLY = 1 OR 2
C   (NEUTRON OR PROTON ORBITALS ONLY). THE CODE ASYRWS SHOULD HAVE
C   PAIRING INPUT APPROPRIATE TO WOODS-SAXON.
C   THE CODE PROBAWS CAN ONLY DERIVE THE MACROSCOPIC CORE QUADRUPOLE
C   MOMENTS (Q0 AND Q2) BECAUSE THE SINGLE PARTICLE QUADRUPOLE MATRIX
C   ELEMENTS ON FILE 17 ARE SET EQUAL TO ZERO.
C
C****
C
C   MODIFICATIONS BY PAUL SEMMES, FEBRUARY 1991
C
C   MAIN CHANGE: IREC INCORPORATED SO THAT J+J-, JZ**2, ETC CAN BE
C   TREATED AS TWO BODY OPERATORS WITH APPROPRIATE
C   PAIRING FACTORS IN ASYRWS

```

```

C
C THE BASIC TWO-BODY TREATMENT OF THE RECOIL TERMS IS GIVEN IN
C NUCL. PHYS. A253 (1975) 45; NOTE, HOWEVER, THAT THE KRONECKER
C DELTAS IN THEIR EQ'N 14 SHOULD BE REMOVED
C
C IF IREC = 1, THEN MATRIX ELEMENTS JPLUS(FINAL,INITIAL),
C JMINUS(F,I) AND JZ(F,I) ARE COMPUTED AND PASSED
C ON TO ASYRWS, WITH FINAL =1,IDIM, INITIAL =1,NU.
C THIS ALLOWS A FULL TWO BODY TREATMENT OF THE TERMS
C JX**2, ETC, INCLUDING 1- AND 3-QUASIPARTICLE
C INTERMEDIATE STATES AND PROPER PAIRING FACTORS
C
C IF IREC = 0, THEN THE RECOIL MATRIX ELEMENTS (J+J+, ETC) ARE
C TREATED AS ONE-BODY OPERATORS
C
C*****
C DESCRIPTION OF THE INPUT
C
C CARD 1: FILE3, FILE17 (FREE FORMAT)
C FILE3 CONTAINS THE DEFORMED S. P. INFO FROM SWGAMMA
C FILE17 IS THE OUTPUT FILE TO BE PASSED TO ASYRWS
C
C 2: IPKT, ISKIP (FREE FORMAT)
C IPKT: THE NUMBER OF DATA SETS (OF A GIVEN
C DEFORMATION AND PARITY) TO BE READ FROM FILE3
C ISKIP: THE FIRST ISKIP DATA SETS ARE NOT USED
C
C 3: IREC (FREE FORMAT)
C IREC = 1: ADDITIONAL CALCULATIONS ARE MADE SO THAT A
C TWO-BODY TREATMENT OF THE RECOIL TERMS IS
C POSSIBLE IN ASYRWS; THE ONE-BODY TREATMENT
C CAN STILL BE SELECTED IN ASYRWS
C
C IREC = 0: ADDITIONAL CALCULATIONS ARE NOT MADE, SO
C ONLY THE ONE-BODY TREATMENT OF THE RECOIL TERMS
C IS POSSIBLE IN ASYRWS
C
C 4: IPAR, NU, (LEVEL(J), J=1,NU) FORMAT: A1,I2,I5I3
C IPAR: '+' OR '-', THE PARITY OF THE DEFORMED SINGLE
C PARTICLE ORBITALS RETAINED FOR THE PARTICLE
C ROTOR CALCULATIONS
C
C NU: THE NUMBER OF ORBITALS RETAINED FOR THE PARTICLE
C ROTOR CALCULATIONS, NU .LE. 15
C
C LEVEL(J): THE ORBITAL NUMBERS, ASSIGNED BY COUNTING
C "FROM THE BOTTOM UP", IE, BY INCREASING ENERGY
C FOR THE PARITY CONSIDERED
C
C NOTE: EACH DEFORMATION SET NEEDS A CARD HERE, EVEN IF
C THAT SET IS SKIPPED.
C IF SKIPPED EG, + 1 1 IS OK

```

```

C
C      5: EMIN, EMAX  FORMAT: 2F10.5
C      THE WAVE FUNCTIONS ARE PRINTED FOR S.P. ORBITALS
C      WITH ENERGIES (IN MEV) WITHIN THE INTERVAL
C      (EMIN, EMAX)
C
C      NOTE: EACH DEFORMATION SET NEEDS A CARD HERE, EVEN IF
C      THAT SET IS SKIPPED.  THUS, FOR DEFORMATION
C      SETS A,B,C, CARDS 1,2,3 ARE FOLLOWED BY
C      4A,5A,4B,5B,4C,5C.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

```

A sample input file (named, e.g., IR179WSD.DAT) that could be appropriate for the prolate states in ¹⁷⁹Ir generated by IR179SWG.DAT is:

```

'SWG10.DAT', 'WSD17.DAT'  FILE3, FILE17
1  0                      IPKT, ISKIP
0                          IREC
-11 14 15 16 17 18 19 20 21 22 23 24  ipar,nu,level(j),j=1,nu
-10.      +0.50              emin,emax                      (for WSDCUP)

```

input file for WSDCUP

Note that the file from SWGAMMA is named here ('SWG10.DAT'), as well as the output file from this code ('WSD17.DAT'). Recall that on a VAX free format character data should be enclosed with apostrophes. These file names must correspond to the files assigned elsewhere; in the case of the SWGAMMA output, this file is assigned most conveniently in the command file (shown later). Note that since IREC=0 is selected here, IREC=0 must be selected in ASYRWS. If however, IREC=1 is chosen here, then IREC=0 can still be selected in ASYRWS. The fourth line of input data (-11 14 15 16 ...) specifies that 11 negative parity orbitals are to be selected for the calculations, and these are the 14th, 15th, 16th, .. etc. orbitals, counted from the bottom up. From the printed output of SWGAMMA, #14 has an energy of -7.0824 MeV, and is the 29th orbital overall, counting from the bottom up. Similarly, #24- has an energy of +0.1942 MeV and is the 48th orbital overall. Since Z=77 for Ir, the proton Fermi level should lie close to orbital #39 overall (corresponding to (Z+1)/2), and this happens to be the 20th positive parity orbital, which has an energy of -2.8172 MeV. This selection of orbitals should include all the negative parity orbitals within about 3 MeV of the Fermi level, and should be quite sufficient for describing the low-lying negative parity states in ¹⁷⁹Ir (if this deformation, etc. is appropriate).

```

C#####
C#####
C#####          PROGRAM ASYRWS          #####
C
C   VERSION: JULY, 1991
C
C   DISTRIBUTED AT THE OAK RIDGE THEORY WORKSHOP, AUG 1991, FOR USE
C   WITH OTHER WOODS-SAXON CODES SWGAMMA (CALCULATES THE DEFORMED
C   S. P. ORBITALS [EIGENVALUES AND EIGENVECTORS]), WSDCUP (COMPUTES
C   THE S. P. MATRIX ELEMENTS [EG, <J+>, ETC] NEEDED FOR ASYRWS), AND
C   PROBAWS (CALCULATES M1/E2 MATRIX ELEMENTS FROM THE PARTICLE +
C   ROTOR EIGENVECTORS GENERATED BY ASYRWS).
C
C   ASYRWS DIAGONALIZES THE PARTICLE + TRIAXIAL ROTOR HAMILTONIAN
C   IN THE STRONG COUPLING BASIS, WITH THE SINGLE-PARTICLE MATRIX
C   ELEMENTS EXPRESSED IN DEFORMED SCHEME. ORIGINAL PROGRAM DESCRIBED
C   IN NUCL. PHYS. A307 (1978) 189. THIS VERSION ACCEPTS INPUT FROM
C   WSDCUP (WOODS-SAXON POTENTIAL).
C
C   SINGLE-PARTICLE ENERGIES AND VARIOUS MATRIX ELEMENTS CALCULATED
C   IN WSDCUP ARE READ FROM FILE17. OUTPUT REQUIRED FOR "TRANSITION
C   PROBABILITY PROGRAM" (PROBAWS) WRITTEN ON FILE18
C
C*****
C
C   MODIFICATIONS BY PAUL SEMMES, FEBRUARY 1991
C
C   INCLUDING:  OPTIONAL TWO BODY TREATMENT OF RECOIL TERMS (J+J-,
C               JZ**2, ETC), WITH APPROPRIATE PAIRING FACTORS
C               K-TRUNCATION
C               EXTENSIONS TO HIGH SPIN (ISPIN .LE. 129)
C               VARIOUS ANGULAR MOMENTUM EXPECTATION VALUES CALCULATED
C               FOR ENERGY EIGENVECTORS
C
C   THE BASIC TWO-BODY TREATMENT OF THE RECOIL TERMS IS DESCRIBED IN
C   NUCL. PHYS. A253 (1975) 45. HOWEVER, NOTE THAT THE KRONECKER
C   DELTAS IN THEIR EQ'N 14 SHOULD BE OMITTED. ALSO, NOTE THAT A
C   SMALL, CONSTANT "CORE CONTRIBUTION" THAT ARISES IN THE TWO-BODY
C   TREATMENT OF THE RECOIL TERMS HAS BEEN OMITTED IN THIS PROGRAM.
C   THIS DOES NOT AFFECT EXCITATION ENERGIES, BUT CAN CAUSE SMALL
C   ERRORS IN THE EXPECTATION VALUES <I.j>, ETC. (IN THE SUBROUTINE
C   "EXPECT") ESPECIALLY NEAR BANDHEADS.
C
C   NOTE THAT THERE IS NO VMI OPTION IN THIS VERSION; THE WOODS-SAXON
C   DEFORMED S.P. STATES ARE WRITTEN IN /N,Nz,LAM,OMEGA> BASIS, NOT
C   THE /N,L,j,OMEGA> BASIS AS IN THE MODIFIED OSCILLATOR VERSION.
C
C#####          #####
C#####
C
C   INPUT DATA (ENERGIES IN MEV):
C

```

C 1. FILE17, FILE18 (FREE FORMAT)
 C FILE17 WAS WRITTEN BY WSDCUP CONTAINS VARIOUS S.P. MATRIX
 C ELEMENTS NEEDED HERE (EG, j+, j-, ETC)
 C FILE18 : NAME OF THE OUTPUT FILE, NEEDED FOR PROBA
 C
 C 2. IPKT, ISKIP (FREE FORMAT)
 C IPKT: NUMBER OF DATA SETS (OF GIVEN DEFORMATION AND PARITY)
 C TO BE READ FROM FILE17
 C ISKIP: THE FIRST ISKIP POINTS ARE NOT USED
 C
 C 3. IREC (FREE FORMAT)
 C IREC=1: TREAT THE RECOIL TERMS (J+J-, J+J+, ETC) AS TWO-
 C BODY OPERATORS, IE, CONSTRUCT THEM FROM MATRIX
 C ELEMENTS OF J+, J-, JZ SUMMED OVER A COMPLETE SET
 C OF INTERMEDIATE STATES (INCLUDING 1- AND 3-QUASI-
 C PARTICLE STATES) EACH WITH ITS CORRECT PAIRING
 C FACTOR
 C IREC=0: TREAT THESE TERMS AS ONE-BODY OPERATORS, AS IN
 C NPA307, 189, WITH SINGLE PARTICLE MATRIX
 C ELEMENTS MULTIPLIED BY UU'+VV'
 C
 C *** RECOMMENDATION: THE IREC=0 OPTION IS SUGGESTED. THE TWO
 C *** APPROACHES SEEM TO GIVE VERY SIMILAR
 C *** RESULTS, AND THE ONE-BODY TREATMENT IS
 C *** SIMPLER. NOTE THAT IF YOU USE IREC=1 HERE,
 C *** IREC=1 MUST HAVE BEEN SELECTED IN WSDCUP.
 C
 C 4. Z, AA, IMIN, ISPIN, KMAX, E2PLUS, E2PLUR (FREE FORMAT)
 C Z: PROTON NUMBER OF THE ODD NUCLEUS, MAY BE EVEN OR ODD.
 C AA: MASS NUMBER OF THE ODD NUCLEUS
 C
 C IMIN: MINIMUM SPIN CONSIDERED IS IMIN/2
 C ISPIN: MAXIMUM SPIN CONSIDERED IS ISPIN/2
 C *** ISPIN .LE. 129 ***
 C *** (ISPIN-IMIN)/2 .LE. 19
 C KMAX: MAX K ALLOWED (FOR TRUNCATION;
 C KMAX = ISPIN => NO TRUNCATION)
 C *** KMAX = ...13, 17, 21, ... KMAX .LE. 29 ***
 C
 C E2PLUS: THE MOMENTS OF INERTIA ARE ASSUMED TO VARY ACCORDING
 C TO THE FORMULA
 C
$$J(K) = 4B \cdot EPS2^{**2} \cdot (\sin(GAMMA + 2K \cdot PI/3))^{**2}$$

 C A. E2PLUS=0 ==> (HBAR)**2/B = 1225/AA**(7/3) (MEV)
 C (GRODZINS' RELATION)
 C B. E2PLUS .GT. 0 ==> THE B-VALUE IS FIXED TO GIVE
 C THIS ENERGY FOR THE LOWEST E2+ OF CORE ROTOR
 C C. E2PLUS .LT. 0 ==> (HBAR**2)/B = (-E2PLUS)/AA**2 (MEV)
 C
 C E2PLUR: FOR E2PLUR .GT. 0 AND E2PLUS .GT. 0 THE GAMMA ANGLE
 C IS CALCULATED TO GIVE THE SECOND 2+ ENERGY OF THE
 C CORE EQUAL TO E2PLUR
 C (NOTE THAT THE CORE GAMMA THUS BECOMES DIFFERENT

FROM THE GAMMA OF THE S.-P. ENERGIES. THIS OPTION
IS NOT RECOMMENDED.)

5. GNO, GN1, IPAIR, CHSI, ETA (FREE FORMAT)
THE PAIRING STRENGTH PARAMETER IS
 $G*A = GNO +/- GN1*(N-Z)/A$; (PROTONS/NEUTRONS)
WITH $SQRT(IPAIR*Z)/SQRT(IPAIR*N)$ ORBITALS INCLUDED ABOVE
AND BELOW THE FERMI LEVEL IN THE PAIRING CALCULATIONS

STANDARD VALUES FOR WOODS-SAXON POTENTIAL, ALL WITH
IPAIR = (Z OR N)/4, WHICHEVER IS ODD
(J. PHYS G6 (1980) 447):

RANGE IN Z	GNO(PROTONS)	GN1(P)	GNO(NEUTRONS)	GN1(N)
Z < 50	17.9	7.4	17.9	7.4
50 = Z, 50 < Z < 88	17.9	0.176*A	18.95	0.078*A
88 = Z, 88 < Z	13.3	0.217*A	19.3	0.084*A

IF IPAIR=99 OR 98 THEN DELTA=GN1/SQRT(AA)
STANDARD: GN1 = 12.
IF IPAIR=99, THE FERMI LEVEL IS SET EQUAL TO GNO IN MEV
IF IPAIR=98, THE FERMI LEVEL IS SET ON TOP OF THE
((Z OR N)/2 + 1) LEVEL

CHSI, ETA: CORIOLIS ATTENUATION PARAMETER
ALL OFF-DIAGONAL S.P. MATRIX ELEMENTS ARE MULTIPLIED BY CHSI.
ETA IS AD HOC POWER ON (UU+VV) (U AND V PAIR FACTORS)
(BUT ETA DOES NOT AFFECT PAIRING FACTORS IN THE TWO BODY
TERMS IF IREC .EQ. 1)

*** NOTE THAT THE ANGULAR MOMENTUM EXPECTATION VALUES (COMPUTED
*** IN SUBROUTINE EXPECT, AFTER ENERGY DIAGONALIZATION) ARE
*** CALCULATED CORRECTLY EVEN IF CHSI .NE. 1., IE, THE SCALING
*** OF THE S.P. MATRIX ELEMENTS (<j+>, ETC) BY CHSI IS REMOVED
*** IN "EXPECT". HOWEVER, IF ETA .NE. 1, THE ATTENUATION OF
*** THESE MATRIX ELEMENTS IS NOT REMOVED, BUT REMAINS IN THE
*** COMPUTED EXPECTATION VALUES <i.j>, ETC.

*** RECOMMENDATION: AVOID CORIOLIS ATTENUATION IF POSSIBLE,
*** BUT IF YOU MUST ATTENUATE USE CHSI.
*** CHSI APPROX 0.7 IS COMMON.

6. IPAR1, NYIC, (LEVEL2(J),J=1,NYIC) FORMAT(A1,I2,I5I3)
IPAR1: PARITY CONSIDERED, "+" OR "-"
NYIC: NUMBER OF ORBITALS CONSIDERED IN THE PARTICLE-ROTOR
CALCULATION, NU .LE. 15
LEVEL2(J): "NUMBERS" ON THE ORBITALS INCLUDED (CALCULATED
FROM THE "BOTTOM" AND FOR THE PARITY "IPAR"
CF. INPUT CARD 7 FOR WSDCUP THE SET OF ORBITALS IN
LEVEL2(J) MUST BE A SUBSET (OFTEN THE FULL SET) OF
ORBITALS LEVEL(J) IN WSDCUP


```

C#####
C#####
C#####          PROGRAM PROBAWS          #####
C
C    VERSION: JULY, 1991
C
C    DISTRIBUTED AT THE OAK RIDGE THEORY WORKSHOP, AUG 1991, FOR
C    USE WITH OTHER WOODS-SAXON CODES, SWGAMMA (CALCULATES THE
C    DEFORMED S.P. ORBITALS [EIGENVALUES AND EIGENVECTORS]),
C    WSDCUP (CALCULATES THE S.P. MATRIX ELEMENTS), AND ASYRWS
C    (DIAGONALIZES THE PARTICLE + ROTOR HAMILTONIAN).
C
C***** PROBAWS CALCULATES M1/E2 MATRIX ELEMENTS IN THE PARTICLE-ROTOR
C    FORMALISM, FROM THE ENERGY EIGENVECTORS SUPPLIED BY ASYRWS.
C    BOTH DIAGONAL AND OFF-DIAGONAL MATRIX ELEMENTS ARE CALCULATED
C    (IE, STATIC MOMENTS AND TRANSITION RATES, MIXING RATIOS, ETC).
C    NOTE THAT SPECTROSCOPIC FACTORS ARE NOT AVAILABLE IN THIS
C    VERSION.
C
C    ORIGINAL PROGRAM WAS PART OF THE PARTICLE-ROTOR PACKAGE
C    DESCRIBED IN NUCL PHYS A307 (1978) 189 AND USED A MODIFIED
C    OSCILLATOR POTENTIAL. THIS VERSION INCORPORATES NUMEROUS
C    CHANGES REQUIRED FOR THE WOODS-SAXON CODES.
C
C    MODIFICATIONS BY PAUL SEMMES, FEBRUARY 1991
C
C    INCLUDING: K TRUNCATION
C               EXTENSION TO HIGH SPINS
C               CALCULATION OF Q0,Q2 MACROSCOPIC MOMENTS FROM
C               THE WOODS-SAXON BETA PARAMETERIZATION
C
C#####          #####
C#####          #####
C
C    INPUT OF SINGLE-PARTICLE QUANTITIES FROM WSDCUP ON FILE17
C    INPUT OF PARTICLE-ROTOR QUANTITIES FROM ASYRWS ON FILE18
C
C    INPUT DATA (PARTLY OVERLAPPING WITH ASYRWS):
C
C    1. FILE17, FILE18 (FREE FORMAT)
C       FILE17: OUTPUT FILE FROM WSDCUP,
C              CONTAINS S.P. MATRIX ELEMENTS
C       FILE18: OUTPUT FILE FROM ASYRWS,
C              CONTAINS ODD-A WAVE FUNCTIONS
C
C    2. IPKT, ISKIP (FREE FORMAT)
C       IPKT: NUMBER OF DATA SETS (OF GIVEN DEFORMATION AND PARITY)
C            TO BE READ FROM FILE17
C       ISKIP: THE FIRST ISKIP SETS (ON FILE17) ARE NOT USED
C
C    3. Z, AA (FREE FORMAT)
C       Z: PROTON NUMBER OF THE ODD-MASS NUCLEUS

```

```

C          (THE PROGRAM DETERMINES WHETHER Z OR N IS ODD)
C      AA: MASS NUMBER OF THE ODD NUCLEUS
C
C      4. CUTOFF, GSFAC, GR (FREE FORMAT)
C          CUTOFF: ENERGY CUTOFF IN keV FOR TRANS. PROB. AND MOMENTS
C          GSFAC: SCALING FACTOR OF THE INTERNAL SPIN G-FACTOR
C              GS(EFF) = GSFAC*GS(FREE);
C              (STANDARD: (0.6 .LE. GSFAC .LE. 0.70)
C          GR : G-FACTOR FOR CORE;
C              IF GR<0 ON INPUT THEN STANDARD VALUE, GR= Z/AA, CHOSEN
C
C          NOTE THAT IMIN, ISPIN & KMAX ARE ALL READ FROM FILE18
C          IMIN : MINIMUM SPIN CONSIDERED IS IMIN/2
C          ISPIN: MAXIMUM SPIN CONSIDERED IS ISPIN/2
C          KMAX : MAXIMUM K CONSIDERED (K TRUNCATION)
C
C      ** NOTE: NONE OF THESE CARDS ARE REPEATED, EVEN IF IPKT .GT. 1 **
C
C*****

```

A sample input file (named, e.g., IR179PR.DAT) that could be appropriate for the prolate states in ¹⁷⁹Ir generated by IR179SWG.DAT, IR179WSD.DAT and IR179ASY.DAT is:

```

'WSD17.DAT', 'ASY18.DAT'      FILE17, FILE18
  1      0                    ipkt,iskip
 77  179                    z,aa
5000. 0.70  -1.              CUTOFF,GSFAC,GR

```

SAMPLE INPUT FILE FOR PROBAWS

Again, note that the input files are appropriately named. All states passed on from ASYRWS (determined there by nant(j)) and within 5000 keV will be used here for the M1/E2 calculations. The spin g-factor (g_s) has been set at 70% of the free g_s value, and the core g-factor g_R will be set to the standard value of Z/AA (since GR < 0 was selected).

All these programs (with the input files given above) could be run with the following simplified command file:

```
$ SET VERIFY
$ SET DEF [youracct.subdir]
$ DELETE RUNWS.LOG;*
$ ASSIGN RUNWS.LOG SYS$OUTPUT
$!
$! RUN SWGAMMA:
$!
$  ASSIGN IR179SWG.DAT FOR$read
$  ASSIGN swg10.DAT FOR010
$  ASSIGN IR179SWG.OUT FOR$PRINT          !FOR PRINT YYY
$    RUN      SWGAMMA
$!
$! RUN WSDCUP:
$!
$  ASSIGN IR179WSD.DAT FOR005
$  ASSIGN IR179WSD.OUT FOR$PRINT          !FOR PRINT YYY
$    RUN      WSDCUP
$!
$! RUN ASYRWS
$!
$  ASSIGN IR179ASY.DAT FOR005
$  ASSIGN IR179ASY.OUT FOR$print          !FOR print, XXX YYY
$    RUN      ASYRWS
$!
$! RUN PROBAWS
$!
$  ASSIGN IR179PR.DAT FOR005
$  ASSIGN IR179PR.OUT FOR$print          !FOR print, XXX YYY
$    RUN      PROBAWS
```

Of course, eventually the default directory should be set (\$ SET DEF [youracct.subdir]) appropriately for your VAX directory! Note that the output file name from SWGAMMA (and containing the information needed for WSDCUP) is assigned in this .COM file, and is then used inside the file IR179WSD.DAT. The other output files passed directly from one program to another are named inside the data files. The output files assigned as FOR\$PRINT contain the printed output for us humans to look at!

The Modified Oscillator Programs:

```

C*****
C#####
C#####
C#####          PROGRAM GAMPN          #####
C#####          #####
C#####          VERSION: JULY, 1991    #####
C#####          #####
C#####          #####
C***    ORIGINAL PROGRAM DESCRIBED IN NUCL PHYS A307 (1978) 189    ****
C              AND PHYSICA SCRIPTA 8 (1973) 17                      *
C                                                                    *
C    PLEASE REPORT ERRORS, INCONSISTENCIES OR PROBLEMS TO:          *
C                                                                    *
C    INGEMAR RAGNARSSON          PAUL SEMMES          *
C    DEPT OF MATH PHYSICS        OR          PHYSICS DEPT, BOX 5051  *
C    LTH, BOX 118                TENNESSEE TECH. UNIV.  *
C    S-22100 LUND, SWEDEN        COOKEVILLE, TN 38505 USA *
C                                                                    *
C                                                                    *
C*****
C
C    VERSION: JULY, 1991
C
C    DISTRIBUTED AT THE OAK RIDGE THEORY WORKSHOP, AUG 1991, FOR USE
C    WITH OTHER MODIFIED-OSCILLATOR CODES ASYRMO (DIAGONALIZES THE
C    PARTICLE + TRIAXIAL ROTOR HAMILTONIAN) AND PROBAMO (CALCULATES
C    M1/E2 MATRIX ELEMENTS FROM THE ENERGY EIGENVECTORS OF ASYRMO)
C
C
C    GAMPN CALCULATES OF SINGLE-PARTICLE ENERGIES AND VARIOUS MATRIX
C    ELEMENTS IN A MODIFIED OSCILLATOR (NILSSON) POTENTIAL.
C    PROGRAM MAINLY DESIGNED TO PROVIDE INPUT FOR SUBSEQUENT ODD-A
C    AND ODD-ODD PARTICLE-ROTOR CALCULATIONS
C
C    SINGLE-PARTICLE TRANSFORMATION: /N 1 j omega> basis --->
C    /N 1 lambda sigma> basis WRITTEN ON FILE2 (NEEDED FOR ODD-ODD
C    CALCULATIONS WITH A PROTON-NEUTRON RESIDUAL INTERACTION)
C
C    DATA FOR VMI CALCULATIONS (IN ASYRMO/ASYRPN) WRITTEN ON FILE16
C    DATA FOR PART-ROTOR PROGRAMS (ASYRPN AND PROBA) WRITTEN ON FILE17
C
C    ALSO POSSIBLE TO CALCULATE ENERGIES IN A CRANKED POTENTIAL
C                                (OMROT .NE. 0)
C
C*****
C
C    DESCRIPTION OF THE INPUT DATA (FREE FORMAT UNLESS SPECIFIED):
C
C    CARD 1. FILE2, FILE16, FILE17
C            OUTPUT FILES TO BE USED FOR SUBSEQUENT APPLICATIONS

```

C (RECALL THAT ON A VAX FREE FORMAT CHARACTER
 C DATA MUST BE ENCLOSED WITH APOSTROPHES)
 C FILE2 CONTAINS THE S.P. WAVE FUNCTIONS IN THE
 C |N,L,LAMBDA,SIGMA> BASIS NEEDED FOR V_{pn} CALCULATIONS
 C FILE16 CONTAINS THE S.P. WAVEFUNCTIONS NEEDED FOR THE VMI
 C OPTION IN ASYR
 C FILE17 CONTAINS THE USUAL OUTPUT NEEDED FOR ASYR, IE,
 C SINGLE PARTICLE MATRIX ELEMENTS LIKE <j+>, <j->, etc
 C
 C 2. ISTRCH, ICORR, IREC
 C ISTRCH=0: CALCULATION IN SPHERICAL COORDINATES
 C (DEF PARAM DELTA2, GAMMAD, DELTA4, DELTA6)
 C ISTRCH=1: CALCULATION IN STRETCHED COORDINATES (STANDARD)
 C (DEF PARAM EPS2, GAMMA, EPS4, EPS6)
 C (NOTE THAT THE SHAPES GENERATED ARE DIFFE-
 C RENT IN THE TWO CASES; FURTHERMORE THE
 C L*S AND L*L TERMS ARE SOMEWHAT DIFFERENT
 C WITH L DEF IN STRETCHED OR SPHER COORDINATES)
 C
 C ICORR=0: NORMAL CALCULATION OF J+/J-/JZ/J+J₋, ETC, IE,
 C APPROXIMATE WITH J+/J-/JZ (STRETCHED)
 C ICORR=1: INCLUDE CORRECTION TERMS FOR J+/J-/JZ FROM THE
 C STRETCHED BASIS (SEE APPENDIX, NUCL PHYS A307,189)
 C AND CONSTRUCT CORRECTED J+J₋, JZ2, ETC FROM THESE
 C
 C IREC = 0: USUAL TREATMENT OF JX2, JY2, JZ2 IN ASYR, IE, AS
 C ONE-BODY OPERATORS WITH UU' + VV' PAIRING FACTORS
 C IREC = 1: "RECOIL" TERMS JX2, JY2, JZ2 ARE TREATED AS TWO-
 C BODY OPERATORS IN ASYRMO => MORE j+, j₋, jz
 C MATRIX ELEMENTS MUST BE CALCULATED HERE (FOR THE
 C SUMS OVER INTERMEDIATE STATES IN ASYRMO)
 C
 C ** RECOMMENDATIONS: FOR NORMAL DEFORMATIONS, THE DIFFERENCES BETWEEN
 C *** THE STRETCHED AND PHYSICAL j+, j₋, jz OPERATORS
 C *** ARE NEGLIGIBLE ==> ICORR=0 IS STANDARD.
 C *** SIMILARLY, THE SIMPLER ONE-BODY TREATMENT OF
 C *** THE RECOIL TERM SEEMS QUITE ADEQUATE ==> IREC=0
 C *** IS STANDARD. (NOTE THAT IF IREC=1 IS SELECTED
 C *** HERE, IREC=0 CAN STILL BE CHOSEN IN ASYRMO.)
 C
 C 3. NKAMY, NNEUPR
 C NKAMY .LE. 0: SAME KAPPA AND MY FOR ALL N-SHELLS
 C NKAMY .GT. 1: DIFFERENT KAPPA AND MY FOR DIFFERENT N-SHELLS
 C (SEE CARD 3 BELOW)
 C FOR NKAMY .GT. 1:(NKAMY-1) .GE. MAX(NPROT,NNEUTR); (CARD 9)
 C (NKAMY-1) .LE. 10
 C NNEUPR=1: CALCULATION FOR PROTONS
 C NNEUPR=-1: CALCULATION FOR NEUTRONS
 C NNEUPR=2: CALCULATION FOR PROTONS AND NEUTRONS (FOR ODD-ODD)
 C
 C 4. KAPPAP(I), MYP(I), KAPPAN(I), MYN(I)
 C OMITTED IF NKAMY .LE. 1; OTHERWISE NKAMY CARDS NEEDED

C KAPPAP AND MYP (KAPPAN AND MYN) VALUES OF L.S AND L**2
 C COUPLING PARAMETERS FOR PROTONS (NEUTRONS) FOR THE
 C DIFFERENT SHELLS, N=0,1,2,3,..., (NKAMY-1)
 C
 C 4A. NKAMYL
 C NUMBER OF N-SHELLS WITH KAPPA AND MY L-DEPENDENT
 C
 C CARDS 3B-3C REPEATED NKAMYL TIMES (OMIT FOR NKAMYL=0):
 C 4B. NSHELL
 C N QUANTUM NUMBER FOR SHELLS WITH L-DEPENDENCE
 C 4C. KAPPAP(N,L), MYP(N,L), KAPPAN(N,L), MYN(N,L)
 C L=0,2,... OR L=1,3,... (N=NSHELL)
 C
 C *** FOR "STANDARD" KAPPA'S & MU 'S, SEE NUCL PHYS A436 (1985) 14 ***
 C
 C 5. KAPPAP, MYP, KAPPAN, MYN
 C THIS CARD MAY NEVER BE OMITTED BUT IS DUMMY FOR NKAMY .GT. 1
 C FOR NKAMY .LE. 1 USED AS CARDS 3 BUT REFERRING TO ALL SHELLS
 C
 C 6. NUU, IPKT, NOYES, ITRANS
 C NUU: NUMBER OF OSCILLATOR SHELLS COUPLED, NUU=4 STAND VALUE
 C (REDUNDANT FOR EPS4=EPS6=OMROT=0 AND ISTRCH=1 BECAUSE
 C THE N-SHELLS ARE PURE IN THIS CASE)
 C IPKT: NUMBER OF DEFORMATIONS, CF. CARD 9 BELOW
 C NOYES=1 IN PART-ROT CALCULATIONS
 C (FOR NOYES=0 ONLY SINGLE PARTICLE ENERGIES BUT NO
 C WAVE-FUNCTIONS OR MATRIX ELEMENTS ARE CALCULATED)
 C ITRANS: CONTROLS OPTION OF TRANSFORMING THE LEVELP(J) AND
 C LEVELN(K) PROTON AND NEUTRON ORBITALS TO THE
 C /N,L,LAM,SIGMA> BASIS (NEEDED IF SUBSEQUENT Vpn
 C CALCULATIONS ARE DESIRED, OUTPUT TO FILE2)
 C ITRANS=0: NO SUCH TRANSFORMATION
 C ITRANS=1: WAVEFUNCTIONS ARE TRANSFORMED, BUT NOT PRINTED
 C ITRANS=2: W.F.'S ARE TRANSFORMED AND PRINTED OUT
 C
 C 7. EMIN, EMAX
 C FOR ENERGIES BETWEEN EMIN AND EMAX (IN OSCILLATOR UNITS) THE
 C WAVE-FUNCTIONS ARE PRINTED
 C
 C 8a. IPARP, NORBP, (LEVELP(J),J=1,NORBP) FORMAT(A1,I2,15I3)
 C IPARP: PARITY CONSIDERED FOR PROTONS, "+" OR "-"
 C NORBP: NUMBER OF PROTON ORBITALS CONSIDERED IN THE
 C PARTICLE-ROTOR CALCULATION, NORBP .LE. 15
 C LEVELP(J): "NUMBERS" ON THE ORBITALS INCLUDED
 C (CALCULATED FROM THE "BOTTOM" AND FOR THE PARITY "IPARP")
 C
 C 8b. IPARN,NORBN,(LEVELN(J),J=1,NORBN)
 C ANALOGOUS TO 7a BUT FOR NEUTRONS
 C
 C 9. Z,A
 C Z: PROTON NUMBER; A: MASS NUMBER
 C FOR Z AND/OR N=A-Z PARTICLES (Z AND A EVEN), THE MICROSCOPIC

```

C          QUADRUPOLE MOMENTS Q0 AND Q2 ARE CALCULATED (WITH A SHARP
C          FERMI SURFACE). AN ASYMMETRY PARAMETER GAMMA CORRESPONDING
C          TO THE MATTER DISTRIBUTION IS THEN DEDUCED
C
C
C          10. IPKT CARDS:
C          EPS2, GAMMA, EPS4, EPS6, OMROT, NPROT, NNEUTR, NSHELP, NSHELN
C              (ISTRCH = 1)
C              OR
C          DELTA2, GAMMAD, DELTA4, DELTA6, OMROT, NPROT, NNEUTR, NSHELP, NSHELN
C              (ISTRCH = 0)
C          FOUR DEFORMATION PARAMETERS
C              (EPS6 (DELTA6) IS NOT DEFINED TO HAVE THE CORRECT
C              TRANSFORMATION PROPERTIES FOR GAMMA .NE. 0 AND SHOULD
C              ONLY BE USED FOR SMALL GAMMA, SAY GAMMA .LE. 15)
C          OMROT: ROTATIONAL FREQUENCY (-0 IN PART-ROTOR CALC)
C          NPROT: NUMBER OF OSCILLATOR SHELLS INCLUDED FOR PROTONS
C          NNEUTR: NUMBER OF OSCILLATOR SHELLS INCLUDED FOR NEUTRONS
C              MAX NUMBER OF SHELLS IN PRESENT VERSION: 10
C          NSHELP, NSHELN: USED IN THE TRANSFORMATION TO /N,L,LAM,SIG>
C              BASIS IF THE N-SHELLS ARE PURE. NSHELP IS THEN THE
C              N-SHELL FOR THE LEVELP(J) PROTON ORBITALS, NSHELN
C              FOR THE LEVELN(K) NEUTRON ORBITALS
C
C*****

```

This program GAMPN provides the single-particle energies, wave functions and matrix elements needed for the odd-A particle + rotor codes ASYRMO and PROBAMO, but has been designed so that it can also be used with a set odd-odd codes that are not described here. Some of the options presented above are important for the odd-odd applications, but are not needed for the odd-A calculations. In particular, FILE2 (input card 1), ITRANS (card 6) and NSHELP, NSHELN (card 10) are used only for odd-odd applications.

The triaxial modified oscillator potential is discussed in detail in S. E. Larsson, Physica Scripta 8 (1973) 17, including the definitions of the oscillator frequencies and the stretched coordinates as used in this program. For quadrupole deformations only (ϵ and γ), using the stretched coordinates removes the coupling between N shells exactly, which is an obvious simplification for numerical calculations. If higher multipoles are included (ϵ_4 , for example) not all couplings between N-shells are removed, but they are reduced, again improving numerical convergence. Thus, the stretched coordinate system generally should be adopted (ISTRCH=1). However, the physical angular momentum operators (j_+ , etc.) are somewhat more complicated in the stretched coordinate system, than in the unstretched. For moderate deformations, the matrix elements of the physical angular momentum operators are nearly identical to the matrix elements of the stretched operators (obtained simply by replacing the spherical angles θ , ϕ with their stretched counterparts). This approximation is made if ICORR=0 is selected, and the additional corrections are carried through if ICORR=1. For most applications, ISTRCH=1 is recommended and ICORR=0 is fully satisfactory. The user should note that if spectroscopic factors are to be calculated in PROBAMO, then the spherical coordinates must be selected here, and the deformation parameters are denoted δ_2 , γ , and δ_4 (instead of ϵ_2 , γ , and ϵ_4 ; note that ϵ and

ϵ_2 are used interchangeably). If only quadrupole deformations are considered (δ_2 , and γ , or ϵ_2 , and γ), then there is an exact correspondence between the shapes of the potential generated by the stretched and unstretched coordinates, and identical calculations can be made with either (as long as sufficient N-shells are included in the unstretched calculation). The (exact) relations between the stretched and unstretched shape parameters for this case are given in J. Phys. G 14 (1988) 1201. However, as soon as higher multipoles are included in the shape parameterization, there is no longer an exact correspondence between the two potentials.

** A note on the shape parameterization: In this code and the following particle + rotor codes, there is no restriction to a particular 60° sector in the (ϵ, γ) plane. The same shape can be obtained with different (ϵ, γ) parameterizations, and generally these differ only by the labeling on the intrinsic axes. For example, an axially symmetric oblate shape can be described by $\epsilon = -0.20$, $\gamma = 0^\circ$, or by $\epsilon = +0.20$, $\gamma = 60^\circ$. [More generally, the shape described by (ϵ, γ) can also be obtained with $(-\epsilon, 60^\circ - \gamma)$.] In the former case, the intrinsic z-axis is the symmetry axis, and Ω will be a good quantum number for the single-particle orbitals, i.e., the $\langle j_z \rangle$ matrix is diagonal. In the latter case, the z-axis is not the symmetry axis, so the $\langle j_z \rangle$ matrix is not diagonal, and the single-particle matrix elements will all look very complicated. Similarly, the particle + rotor eigenfunctions will look much more complicated in the latter case, but all energies, M1/E2 matrix elements, etc. will be completely identical. Clearly, the wave functions are simpler to understand and interpret if the oblate nuclear shape is described by the $\epsilon = -0.20$, $\gamma = 0^\circ$ parameterization. For this reason, it is convenient to adopt the following convention for describing nuclear shapes:

$\epsilon > 0.$, $\gamma = 0.$	for axially symmetric prolate shapes
$\epsilon > 0.$, $0. < \gamma \leq 30.$	for "prolatish" triaxial shapes
$\epsilon < 0.$, $0. < \gamma \leq 30.$	for "oblatish" triaxial shapes
$\epsilon < 0.$, $\gamma = 0.$	for axially symmetric oblate shapes

Note that this convention is a matter of convenience only, and is not required by this or the following Modified Oscillator particle + rotor codes.

Other than specifying the deformation, the most important parameters that the user must provide are the κ 's and μ 's that determine the strengths of the $l \cdot s$ and $l \cdot l$ terms in the modified oscillator potential. The safest (and recommended) approach is to adopt a "standard" set of N-dependent κ 's and μ 's, and not try to adjust them to fit your particular application. A lot of nuclear physics lore is built into these parameters, and while a "slight adjustment of the single particle energies" often seems to improve the quality of a particular calculation, usually such adjustments are not unique, and the desired improvements can be achieved by other means which are far more justified physically. The parameter NKAMYL (card 4a) allows a very flexible adjustment of the single-particle energies, but its use is NOT recommended here. The "standard set" of κ and μ parameters recommended here and listed in the sample input file below, are given in T. Bengtsson and I. Ragnarsson, Nucl. Phys. A436 (1985) 14. An "improved set" for the proton parameters in the $A \approx 130$ region has been proposed by J. Y. Zhang et al., Phys. Rev. C39 (1989) 714, and some evidence exists that the standard set needs to be improved in the actinide region (R. Bengtsson, et al. Physica Scripta 39 (1989) 196). Note that both proton and

neutron parameters are required, and GAMPN selects the appropriate set according to the value of NNEUPR (input card 3). Similarly, NNEUPR controls whether card 8a or 8b is used to select the Nilsson orbitals that are retained for generating the single-particle matrix elements needed by ASYR and PROBA (and constructing the strong coupling basis states there). For the odd-A particle + rotor applications, either the proton (NNEUPR=1) or the neutron (NNEUPR=-1) calculations should be made, but not both.

A sample input file (named, e.g., GAMIR.DAT) that could be appropriate for the negative parity states of ^{179}Ir is given below:

```
'for002.dat' 'for016.dat' 'for017.dat'      file2, file16, file17
1,0,1                      ISTRCH,ICORR,irec
9,1                        NKAMY,NNEUPR
0.120,0.00,0.120,0.00      'STANDARD' KAPPA, MU'S PROTON AND NEUTRON, N=0
0.120,0.00,0.120,0.00      KAPPA(PROT),MU(PROT),KAPPAN(NEUT),MU(NEUT) N=1
0.105,0.00,0.105,0.00      KAPPAP, MUP, KAPPN, MUN                      N=2
0.090,0.30,0.090,0.25      KAPPAP, MUP, KAPPN, MUN                      N=3
0.065,0.57,0.070,0.39                        N=4
0.060,0.65,0.062,0.43                        N=5
0.054,0.69,0.062,0.34                        N=6
0.054,0.69,0.062,0.26                        N=7
0.054,0.69,0.062,0.26                        N=8
0
                                NKAMYL
0.054,0.69,0.062,0.26
0,1,1,0                      NUU,IPKT,NOYES,ITRANS
5.5,7.0                      EMIN,EMAX
-11 14 15 16 17 18 19 20 21 22 23 24 25      IPARP, NORBITP, LEVELP
+ 7 23 24 25 26 27 29 32 28 29 30 31 32      IPARN, NORBITN, LEVELN
78,180                          Z,A
0.240,00., 0.00,0.,0.0000,8,8,0,0
0.190,20., 0.00,0.,0.0000,7,7,0,0
(LAST CARD: EPS,GAMMA,EPS4,EPS6,OMROT,NPROT,NNEUTR, NSHELP,NSHELN)
1234567890123456789012345678901234567890
SAMPLE INPUT FILE FOR GAMPN
*****
```

Note that 9 oscillator shells (N=0,1,2, ...,8) are included in the calculation, even though the orbitals of interest are from the N=5 shell and no coupling between the N-shells is present (because NUU=0 prevents it, but there is none anyway since ISTRCH=1 and only quadrupole deformations are included). Even so, it is important to include enough N-shells to generate a sufficient number of single-particle energies for the BCS calculation done in ASYR. Both positive and negative parity calculations are done by the code, even though only the negative parity states are retained for ASYR. The single-particle energies of the positive parity states are needed for the later BCS calculation (if λ and Δ are derived). Also note that the maximum N-shell actually used in the diagonalization is specified by NPROT or NNEUTR in "card 10", and this has been set to NPROT=8 to ensure sufficient positive parity states are generated. Two cards with deformations, etc. are shown, but only the first is read since IPKT=1. Multiple calculations (i.e., for different deformations) could be selected with IPKT > 1, and then IPKT cards specifying the deformations would be needed.

Finally, on card 8a, 11 negative parity orbitals are selected, and these are the 14th, 15th, ... 24th negative parity Nilsson orbitals generated at this deformation, and counted "from the bottom up" (i.e., by increasing energy). Generally, a sufficient number of orbitals should be included to ensure numerical convergence in ASYR, and typically 5 above and 5 below the Fermi level are more than enough. A maximum of 15 is allowed.

```

C#####
C#####
C#####          PROGRAM ASYRMO          #####
C#####          #####
C#####          #####
C
C  VERSION: JULY 1991
C
C  DISTRIBUTED AT THE OAK RIDGE THEORY WORKSHOP, AUG 1991, FOR
C  USE WITH OTHER MODIFIED OSCILLATOR CODES, GAMPN (CALCULATES
C  THE DEFORMED SINGLE PARTICLE ORBITALS, THEIR EIGENVALUES,
C  EIGENVECTORS, AND THE S. P. MATRIX ELEMENTS NEEDED FOR ASYRMO,
C  EG, <J+>, ETC) AND PROBAMO (COMPUTES THE M1/E2 MATRIX ELEMENTS
C  FROM THE PARTICLE + ROTOR EIGENVECTORS GENERATED IN ASYRMO).
C
C
C  ASYRMO DIAGONALIZES THE PARTICLE + TRIAXIAL ROTOR HAMILTONIAN
C  IN THE STRONG COUPLING BASIS, WITH THE S. P. MATRIX ELEMENTS
C  EXPRESSED IN DEFORMED SCHEME. ORIGINAL PROGRAM DESCRIBED IN
C  NUCL. PHYS. A307 (1978) 189. THIS VERSION ACCEPTS INPUT FROM
C  GAMPN (MODIFIED OSCILLATOR POTENTIAL).
C
C  SINGLE-PARTICLE ENERGIES AND VARIOUS MATRIX ELEMENTS AS
C  CALCULATED IN GAMPN ARE READ FROM FILES 16 AND 17. OUPUT DATA
C  FOR M1/E2 MATRIX ELEMENTS, ETC (PROBAMO) WRITTEN ON FILE18
C
C*****
C
C  NUMEROUS MODIFICATIONS FROM THE ORIGINAL DESCRIPTION HAVE BEEN
C  MADE, INCLUDING:
C      OPTIONAL TWO-BODY TREATMENT OF THE RECOIL TERMS
C      K-TRUNCTION
C      EXTENSIONS TO HIGH-SPIN (BUT STILL ONLY 1-QP STATES)
C      VARIOUS ANGULAR MOMENTUM EXPECTATION VALUES CALCULATED
C          FOR THE ENERGY EIGENVECTORS
C      POSSIBLE VMI (VARIABLE MOMENT OF INERTIA) TREATMENT OF
C          EVEN-EVEN CORE SPECTRUM (BY AUSTYN GRIFFITHS)
C
C  THE BASIC TWO-BODY TREATMENT OF THE RECOIL TERMS (J+J-, JZ**2, ETC)
C  IS DESCRIBED IN NUCL PHYS A253 (1975) 45. HOWEVER, NOTE THAT THE
C  KRONECKER DELTAS IN THEIR EQN 14 SHOULD BE OMITTED. ALSO, NOTE THAT
C  A SMALL, CONSTANT "CORE CONTRIBUTION" THAT ARISES IN THE TWO-BODY
C  TREATMENT HAS BEEN OMITTED HERE. THIS DOES NOT AFFECT EXCITATION
C  ENERGIES, BUT CAN CAUSE SMALL ERRORS IN THE EXPECTATION VALUES
C  <I.j>, ETC (IN THE SUBROUTINE "EXPECT") ESPECIALLY NEAR BANDHEADS.
C
C  THE VMI TREATMENT FOR THE CORE ENERGY SPECTRUM IS INCORPORATED
C  BY THE METHOD OF NUCL PHYS A253 (1975) 231. THE VMI CORE
C  PARAMETERIZATION IS ALSO GIVEN THERE (INCLUDING TRIAXIAL SHAPES),
C  AND FOR AXIALLY SYMMETRIC SHAPES, THIS IS EQUIVALENT TO THE USUAL
C  METHODS (PHYS REV 178 (1969) 1864)
C
C*****

```

C
C INPUT DATA (ENERGIES IN MEV):
C
C 1. FILE16, FILE17, FILE18 (FREE FORMAT)
C FILE16, FILE17 WERE WRITTEN BY GAMPN AND ARE INPUT FILES.
C THESE CONTAIN THE S.P. WAVEFUNCTIONS (FILE16, NEEDED
C HERE IF THE VMI OPTION IS EXERCISED) AND VARIOUS S.P.
C QUANTITIES NEEDED HERE (EG, MATRIX ELEMENTS OF $j+$ ETC)
C FILE18 : NAME OF THE OUTPUT FILE, NEEDED FOR PROBAMO
C
C 2. IPKT, ISKIP (FREE FORMAT)
C IPKT: NUMBER OF DATA SETS (OF GIVEN DEFORMATION AND PARITY)
C TO BE READ FROM FILE17
C ISKIP: THE FIRST ISKIP SETS ARE NOT USED
C
C 3. ISTRCH, IREC (FREE FORMAT)
C ISTRCH=0: CALCULATION IN SPHERICAL COORDINATES
C (DEF PARAM DELTA2, GAMMAD, DELTA4, DELTA6)
C ISTRCH=1: CALCULATION IN STRETCHED COORDINATES (STANDARD)
C (DEF PARAM EPS2, GAMMA, EPS4, EPS6)
C
C IREC=1: TREAT THE RECOIL TERMS ($J+J-$, $J+J+$, JZ^2 , ETC) AS
C TWO BODY TERMS, IE, CONSTRUCT THEM FROM MATRIX
C ELEMENTS OF $J+$, $J-$, JZ SUMMED OVER A COMPLETE SET
C OF INTERMEDIATE STATES (INCLUDING 1-QP AND 3-QP
C STATES), EACH TERM WITH ITS CORRECT PAIRING FACTOR
C IREC=0: TREAT THESE TERMS AS ONE-BODY OPERATORS, AS IN
C NPA307, 189 WITH SINGLE PARTICLE MATRIX ELEMENTS
C MULTIPLIED BY $UU'+VV'$
C
C *** RECOMMENDATION: THE IREC=0 OPTION IS SUGGESTED. THE TWO
C *** APPROACHES SEEM TO GIVE VERY SIMILAR
C *** RESULTS, AND THE ONE-BODY TREATMENT IS
C *** SIMPLER. NOTE THAT IF YOU USE IREC=1 HERE,
C *** IREC=1 MUST HAVE BEEN SELECTED IN GAMPN.
C
C 4. VMI, NMIN, NMAX, IARCUT, A00, STIFF (FREE FORMAT)
C VMI=1 : CALCULATION OF CORE STATES WITH VMI
C NMIN, NMAX : MINIMUM/MAXIMUM N-SHELL IN DEFORMED S.P.
C WAVEFUNCTIONS
C IARCUT: NUMBER OF CORE STATES INCLUDED FOR EACH (CORE) SPIN
C A00, STIFF : VMI PARAMETERS (MEV AND MEV^{**3})
C $A00=1/(2*J0)$, $STIFF=C-1/(2*J1)$
C WHERE J0 AND C ARE THE VMI PARAMETERS OF
C MARISCOTTI ET AL, PHYS REV 178 (1969) 1864.
C ALSO, J0 AND J1 ARE THE USUAL HARRIS PARAMETERS,
C OBTAINED BY FITTING $J(\text{MOM OF INERTIA})$ VS. hw^{**2}
C $SOFTNESS=1/(2*STIFF**THETA_00**3)$
C
C STANDARD: VMI=0. FOR MOST APPLICATIONS, THE RIGID ROTOR CORE
C IS SUFFICIENT.
C

C 5. Z, AA, IMIN, ISPIN, KMAX, E2PLUS, E2PLUR (FREE FORMAT)
 C Z: PROTON NUMBER OF THE ODD-MASS NUCLEUS, MAY BE EVEN OR ODD.
 C AA: MASS NUMBER OF THE ODD NUCLEUS
 C
 C IMIN: MINIMUM SPIN CONSIDERED IS IMIN/2
 C ISPIN: MAXIMUM SPIN CONSIDERED IS ISPIN/2
 C *** ISPIN .LE. 129 ***
 C *** (ISPIN-IMIN)/2 .LE. 19
 C
 C KMAX: MAX K ALLOWED (FOR TRUNCATION;
 C KMAX = ISPIN => NO TRUNCATION)
 C *** KMAX = ...13, 17, 21, ... KMAX .LE. 29 ***
 C
 C E2PLUS: THE MOMENTS OF INERTIA ARE ASSUMED TO VARY ACCORDING
 C TO THE FORMULA
 C
$$J(K) = 4B \cdot EPS2^{**2} \cdot (\sin(GAMMA + 2K \cdot PI/3))^{**2}$$

 C A. E2PLUS=0 ==> $(HBAR)^{**2}/B = 1225/AA^{**2}(7/3)$ (MEV)
 C (GRODZINS' RELATION)
 C B. E2PLUS .GT. 0 ==> THE B-VALUE IS FIXED TO GIVE
 C THIS ENERGY FOR THE LOWEST 2+ OF CORE ROTOR
 C C. E2PLUS .LT. 0 ==> $(HBAR^{**2})/B = (-E2PLUS)/AA^{**2}$ (MEV)
 C
 C E2PLUR: FOR E2PLUR .GT. 0 AND E2PLUS .GT. 0 THE GAMMA ANGLE
 C IS CALCULATED TO GIVE THE SECOND 2+ ENERGY OF THE
 C CORE EQUAL TO E2PLUR
 C (NOTE THAT THE CORE GAMMA THUS BECOMES DIFFERENT
 C FROM THE GAMMA OF THE S.-P. ENERGIES. THIS OPTION
 C IS NOT RECOMMENDED.)
 C
 C 6. GN0, GN1, IPAIR, CHSI, ETA (FREE FORMAT)
 C THE PAIRING STRENGTH PARAMETER IS
 C $G \cdot A = GN0 \pm GN1 \cdot (N-Z)/A$; (PROTONS/NEUTRONS)
 C WITH $SQRT(IPAIR \cdot Z)/SQRT(IPAIR \cdot N)$ ORBITALS INCLUDED ABOVE
 C AND BELOW THE FERMI LEVEL IN THE PAIRING CALCULATIONS
 C
 C STANDARD: GN0 = 19.2, GN1 = 7.4, IPAIR = 15
 C (NUCL PHYS A131 (1969) 1)
 C IF (Z .LT. 60 OR N .LT. 60):
 C GN0=22.0, GN1=8.0, IPAIR=5
 C (E. G. PHYS SCRIPTA 29 (1984) ...)
 C
 C IF IPAIR=99 OR GN0=0. THEN DELTA=GN1/SQRT(AA)
 C STANDARD: GN1 = 12.
 C IF IPAIR=99, THE FERMI LEVEL IS SET EQUAL TO GN0 IN MEV
 C IF GN0=0., THE FERMI LEVEL IS SET ON TOP OF THE
 C (Z OR N)/2 + 1 LEVEL
 C
 C CHSI, ETA: CORIOLIS ATTENUATION PARAMETER
 C ALL (OFF-DIAGONAL) S.P. MATRIX ELEMENTS ARE MULTIPLIED BY CHSI
 C ETA IS AD HOC POWER ON (UU+VV) (U AND V PAIR FACTORS)
 C (BUT ETA DOES NOT AFFECT THE PAIRING FACTORS IN THE TWO-BODY
 C TERMS IF IREC = 1)

```

C
C *** NOTE THAT THE ANGULAR MOMENTUM EXPECTATION VALUES (COMPUTED
C *** IN THE SUBROUTINE "EXPECT", AFTER THE ENERGY DIAGONALIZATION)
C *** ARE CALCULATED CORRECTLY EVEN IF CHSI .NE. 1, IE, THE SCALING
C *** OF THE S.P. MATRIX ELEMENTS (<j+>, ETC) BY CHSI IS REMOVED
C *** IN "EXPECT". HOWEVER, IF ETA .NE. 1, THE ATTENUATION OF
C *** THESE MATRIX ELEMENTS IS NOT REMOVED, BUT REMAINS IN THE
C *** COMPUTED EXPECTATION VALUES <I.j>, ETC.
C
C *** RECOMMENDATION: AVOID CORIOLIS ATTENUATION IF POSSIBLE,
C *** BUT IF YOU MUST ATTENUATE, USE CHSI.
C *** CHSI APPROX 0.7 IS COMMON.
C
C 7. IPAR1, NYIC, (LEVEL2(J),J=1,NYIC)      FORMAT(A1,I2,15I3)
C      IPAR1: PARITY CONSIDERED, "+" OR "-"
C      NYIC: NUMBER OF ORBITALS CONSIDERED IN THE PARTICLE-ROTOR
C            CALCULATION, NU .LE. 15
C      LEVEL2(J): "NUMBERS" ON THE ORBITALS INCLUDED (CALCULATED
C                  FROM THE "BOTTOM" AND FOR THE PARITY "IPAR"
C                  CF. INPUT CARD 7 FOR GAMPN THE SET OF ORBITALS IN
C                  LEVEL2(J) MUST BE A SUBSET (OFTEN THE FULL SET) OF
C                  ORBITALS LEVEL(J) IN GAMPN
C
C 8. NANTJ(I), I=1,20 (FREE FORMAT)
C      NUMBER OF STATES TO BE CALCULATED FOR I=IMIN/2, ..., IMAX/2
C      AND TO BE WRITTEN TO FILE18, AND THUS PASSED ON TO PROBAMO.
C      PROBAMO CURRENTLY ALLOWS UP TO 60 STATES TOTAL.
C      (FOR SMALL VALUES OF ISPIN, THE LAST NUMBERS ARE REDUNDANT)
C      ***** NANT(J) .LE. 10 *****
C
C 9. NOUTJ(I), I=1,20 (FREE FORMAT)
C      NUMBER OF STATES AT SPIN I=IMIN/2, ..., IMAX/2
C      FOR WHICH THE WAVE-FUNCTIONS ARE PRINTED
C      (NOUTJ(I) .LE. NANTJ(I))
C
C 10. IPOUT,IPOUT(I) I=1,20 (FREE FORMAT)
C      IPOUT .NE. 0 :CORE STATES PRINTED
C      IPOUT(I)      :NUMBER OF STATES AT SPIN I=2, 3, ....., 20
C      FOR WHICH THE CORE TRIAXIAL ROTOR WAVE-FUNCTIONS ARE PRINTED
C
C ** NOTE: NONE OF THESE CARDS ARE REPEATED, EVEN IF IPKT .GT. 1 **
C
C*****

```

A sample input file (e.g., named ASYIR.DAT) that could be appropriate for ^{179}Ir with the GAMPN input file GAMIR.DAT is shown below:

```
'FOR016.DAT' 'FOR017.DAT' 'FOR018.DAT'      FILE16,FILE17,FILE18
1,0                                             IPKT,ISKIP
1,0                                             ISTRCH,IRES
1,5,5,8,0.0188366,0.0026628                 VMI,NMIN,NMAX,IARCUT,A00,STIFF
77,179,1,29,29,0.110,0.0                     Z,AA,IMIN,ISPIN,KMAX,E2PLUS,E2PLUR
19.2,7.4,15,1.0,1.0                           GNO,GN1,IPAIR,CHSI,ETA
-11 14 15 16 17 18 19 20 21 22 23 24         IPAR1,NYIC,(LEVEL2(J),J=1,NYIC)
  1  1  3  3  3  2  2  2  2  2  2  2  2  3  3  1  1  1  1  1  1  NANT(J)
  1  1  2  2  2  2  2  2  2  2  2  2  2  3  3  1  1  1  1  1  1  NOUT(J)
  1  2  1  1  0  1  0  1  0  1  0  1  0  1  0  1  0  1  0  0  0  IPOUT(I)
1234567890123456789012345678901234567890
SAMPLE INPUT FILE FOR ASYRMO
*****
```

First, note that the input files from GAMPN have the same names as in GAMIR.DAT. Also, VMI=1 indicates that the VMI option is to be used, and so the rest of the input on the fourth line is important. Since the Nilsson states of interest have only components with $N=5$, $NMIN=NMAX=5$ is selected. The VMI parameters A00 and STIFF were derived from the Harris parameters J_0 and J_1 , which were determined from a fit of the moment of inertia in the core (taken as ^{180}Pt) vs. $(\hbar\omega)^2$. (See M. J. A. de Voigt et al., Rev. Mod. Phys. 55 (1983) 949 for definitions and examples, and see M. A. J. Mariscotti et al., Phys. Rev. 178 (1969) 1864 for the original VMI discussion and its relation to the Harris parameters. In the case of ^{180}Pt , the Harris plot is not linear at low spins due to shape coexistence effects, and the parameters used here were derived from the higher spin region, $R=6$ to 16.) Some care must be used when the VMI option is used, especially in regions where shape coexistence is suspected. For most applications, the rigid rotor core is fully sufficient, and thus VMI=0 should be selected. Also note that using the VMI implies a one-body treatment for the recoil term, but it is still possible to define (and use) the Coriolis attenuation option with either chsi (ζ) or eta (η). Neither is used here, and generally, Coriolis attenuation should be avoided as much as possible. Note that the same set of Nilsson orbitals selected in GAMIR.DAT is also selected here, but only a subset of GAMPN's orbitals is required here, not necessarily the full set. Finally, note that the "standard" BCS treatment of pairing is used here, with GNO and GN1 set at their recommended values.


```

C#####
C#####
C#####          PROGRAM PROBAMO          #####
C
C    VERSION: JULY, 1991
C
C    DISTRIBUTED AT THE OAK RIDGE THEORY WORKSHOP, AUG 1991, FOR
C    USE WITH OTHER MODIFIED-OSCILLATOR CODES, GAMPN (CALCULATES
C    THE DEFORMED SINGLE PARTICLE ORBITALS, THEIR EIGENVALUES,
C    EIGENVECTORS, AND THE S.P. MATRIX ELEMENTS NEEDED LATER, EG,
C    <j+>, ETC), AND ASYRMO (DIAGONALIZES THE PARTICLE + TRIAXIAL
C    ROTOR HAMILTONIAN).
C
C#####          #####
C#####
C
C***** PROBAMO CALCULATES M1/E2 MATRIX ELEMENTS IN THE PARTICLE-ROTOR
C    FORMAILISM FROM THE ENERGY EIGENVECTORS SUPPLIED BY ASYRMO.
C    BOTH DIAGONAL AND OFF-DIAGONAL MATRIX ELEMENTS ARE CALCULATED
C    (IE, STATIC MOMENTS, TRANSITION RATES, MIXING RATIOS, ETC).
C
C    SPECTROSCOPIC FACTORS FOR SINGLE NUCLEON TRANSFER REACTIONS
C    CAN ALSO BE CALCULATED, AS WELL AS THE HYPERFINE ANOMALIES
C    (DUE TO THE DISTRIBUTION OF MAGNETIZATION INSIDE THE NUCLEUS;
C    SEE PHYS REV 123 (1961) 1326)
C
C*****
C
C    INPUT OF SINGLE-PARTICLE QUANTITIES FROM GAMPN ON FILE17
C    INPUT OF PARTICLE-ROTOR QUANTITIES FROM ASYRMO ON FILE18
C
C    INPUT DATA (PARTLY OVERLAPPING WITH ASYRMO):
C
C    CARD 1. FILE17, FILE18 (FREE FORMAT)
C             FILE17: OUTPUT FILE FROM GAMPN,
C                   CONTAINS S.P. MATRIX ELEMENTS
C             FILE18: OUTPUT FILE FROM ASYRMO,
C                   CONTAINS ODD-A WAVE FUNCTIONS
C
C    2. IPKT, ISKIP (FREE FORMAT)
C       IPKT: NUMBER OF DATA SETS (OF GIVEN DEFORMATION AND PARITY)
C            TO BE READ FROM FILE17
C       ISKIP: THE FIRST ISKIP SETS (ON FILE17) ARE NOT USED
C
C    3. ISTRCH (FREE FORMAT)
C       ISTRCH=0: CALCULATION IN SPHERICAL COORDINATES
C                (DEF PARAM DELTA2, GAMMAD, DELTA4, DELTA6)
C       ISTRCH=1: CALCULATION IN STRETCHED COORDINATES (STANDARD)
C                (DEF PARAM EPS2, GAMMA, EPS4, EPS6)
C
C    4. Z, AA (FREE FORMAT)
C       Z: THE PROTON NUMBER OF THE ODD-MASS NUCLEUS

```

```

C      AA: MASS NUMBER OF THE ODD NUCLEUS
C
C      5. ISPEC, CUTOFF, IQ, GSFAC, GR  (FREE FORMAT)
C      ISPEC: CONTROLS CALCULATION OF SPECTROSCOPIC FACTORS;
C      ISPEC=0 - NO SPEC. FACTORS CALCULATED
C      ISPEC=1 - CALCULATE SPEC. FACTOR IF ISTRCH=0 ALSO
C
C      CUTOFF: ENERGY CUTOFF IN keV FOR TRANS. PROB. AND MOMENTS
C
C      IQ=0 - MACROSCOPIC CALC OF QUADRUPOLE MOMENTS FOR CORE
C              (FROM A HOMOGENOUS SHARP SURFACE BODY)
C      IQ=1 - THE CORE QUADR MOMENTS ARE CALCULATED FROM THE SINGLE
C              PARTICLE MOMENTS ASSUMING A SHARP FERMI SURFACE
C      FOR ODD-NEUTRON NUCLEUS, IQ=0 MUST BE USED
C
C      GSFAC: SCALING FACTOR OF THE INTERNAL SPIN G-FACTOR
C      GS(EFF) = GSFAC*GS(FREE);
C              (STANDARD: (0.6 .LT. GSFAC .LT. 1.0))
C      GR : G-FACTOR FOR CORE;
C              IF GR<0 ON INPUT THEN STANDARD VALUE, GR= Z/AA, CHOSEN
C
C      NOTE THAT IMIN, ISPIN & KMAX ARE ALL READ FROM FILE18
C      IMIN : MINIMUM SPIN CONSIDERED IS IMIN/2
C      ISPIN: MAXIMUM SPIN CONSIDERED IS ISPIN/2
C      KMAX : MAXIMUM K CONSIDERED (K TRUNCATION)
C
C      6. BS2(S-STATE), BS4(S-STATE), BS2(P-STATE), BS4(P-STATE)
C      (FREE FORMAT)
C      THE FACTORS OF R**2 AND R**4 FOR THE SPIN-OPERATOR
C      WHEN CALCULATING THE HYPERFINE ANOMALY.
C      GIVEN FOR ELECTRONIC S- AND P-STATE
C      IF (BS2(I) .EQ. 0) NO CALCULATION OF HYPERFINE ANOMALIES
C
C*****

```

A sample input file (e.g., named PROBIR.DAT) that could be appropriate for ¹⁷⁹Ir with the previous input files is shown below:

```

'FOR017.DAT' 'FOR018.DAT'      FILE17,FILE18
1,0                             ipkt,iskip
1                               isrtch
77,179                         Z,AA
0,2300.,0,0.60,-1.            ISPEC,CUTOFF,IQ,GSFAC,GR
0.0000, 0.000,0.000, 0.000    BS2,BS4 (FOR S-STATE), BS2,BS4(P-STATE)
SAMPLE INPUT FILE FOR PROBAMO
*****

```

Note that the input files from GAMPN and ASYRMO are named appropriately. All states passed on by ASYRMO (determined there by nant(j)) and within 2300 keV of the lowest state will be included here in the M1/E2 calculations. Spectroscopic factors are not requested here (ISPEC=0), and could not be calculated at this point anyway with ISTRCH=1. In PROBAMO, the core E2 moments

can be obtained either from the "macroscopic" nuclear shape (defined by the deformation parameters, and using a sharp surface) or microscopically, by summing up the single particle matrix elements q_{22} and q_{20} generated in GAMPN. (The microscopic definition can be used only if the proton orbitals were generated in GAMPN, i.e., if this calculation is for an odd-Z nucleus.) Generally, these two definitions give similar, but not identical results. It is recommended here to use the macroscopic moments ($IQ=0$) as selected here. Also, ISTRCH is important here, because the macroscopic moments are calculated slightly differently for stretched and unstretched coordinates. Note that the spin g-factor (g_s) has been chosen at 60% of the free value (60% or 70% is standard), and the standard estimate for the core g-factor is selected with $g_R < 0$ (standard estimate: $g_R = Z/A$). Finally, no calculation of the hyperfine anomalies is requested (and this is standard).

All these programs (with the input files given above) could be run with the following simplified command file:

```
$ SET VERIFY
$ SET DEF [youracct.subdir]
$ DELETE RUNMO.LOG;*
$ ASSIGN RUNMO.LOG SYS$OUTPUT
$!      THIS DCL RESIDES IN "[semmes.ornl]RUNMO.COM".
$! RUN GAMPN:
$!
$   ASSIGN GAMIR.DAT FOR005
$   ASSIGN GAMIR.OUT FOR$PRINT          !FOR PRINT YYY
$       RUN      GAMPN
$!
$! RUN ASYRMO
$!
$   ASSIGN ASYIR.DAT FOR005
$   ASSIGN ASYIR.OUT FOR$print          !FOR print, XXX YYY
$       RUN      ASYRMO
$!
$! RUN PROBAMO
$!
$   ASSIGN PROBIR.DAT FOR005
$   ASSIGN PROBIR.OUT FOR$print          !FOR print, XXX YYY
```

Of course, eventually the default directory should be set (\$ SET DEF [youracct.subdir]) appropriately for your VAX directory! Note that all the data files that the user must set up are assigned as FOR005, and all the printed output files are assigned as FOR\$PRINT. The other input files that are generated by the programs are specified inside the data files.

Final remarks

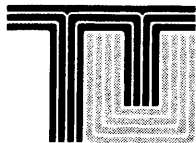
This manual was written with the intent of providing a novice user essentially all the basic information needed to use these computer codes wisely and to understand the main features of the particle + rotor model, warts and all. Before leaving you to your future happy computing experiences (or perhaps the wart medicine), it is important to emphasize a few fundamental restrictions of this model:

1. The basis states are restricted to 1 quasiparticle + a collective rotor core. This model, in its present form, cannot be applied to high-spin states where alignment of "core nucleons" takes place. The necessary 3-qp states are simply not included here.

2. The underlying core is assumed to be rigid, in the sense that a static deformed shape must be a sufficiently realistic description of the mean field experienced by the unpaired particle. A non-rigid core energy spectrum can be accommodated in the Modified Oscillator version through the VMI option, but this does not give a fully consistent description of the changing properties of the core because other possible variations (e.g., shape, pairing field, etc.) are not included. No shape vibrations are included, and only a single fixed shape can be treated (no shape coexistence).

Keeping these restrictions in mind will help ensure the fruitful use of these codes, and may lead to improved formulations of the model.

Good Luck!



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March 3, 1993

Dr. Andrew Stuchbery
Department of Nuclear Physics
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Canberra ACT 2601, Australia

Hello Andrew,

Enclosed is a manual that describes the particle + triaxial rotor programs. The programs and sample input files have been sent by email, so you should have them by now. There are two different packages of programs, one that uses the Modified Oscillator Potential, and another that uses the Woods-Saxon. For the most part, these two sets are very similar in terms of what can be calculated and the way the input and output is structured, but some technical differences remain because the single particle basis used to describe the Nilsson orbitals is different in the two cases. Also, due to the structure of the code SWGAMMA, there is a particular choice for the β and γ deformations that must be made for particle-rotor applications (i.e., a particular 60° sector of the β, γ plane that is used to represent the "collective sector"). The modified oscillator codes are not restricted like that, but recall that a particle-rotor model assumes a collective rotor core, so it is not directly possible to make a calculation with these programs that would correspond to a cranking description "outside the collective sector". The restrictions on β and γ in the Woods-Saxon programs is described on page 10 of the manual. Finally, the bulk of the manual is just a reprint of the documentation found at the beginning of each program, so even if the manual is eaten by the dog essentially all the information is given in the comments inside the programs. Good luck!

Regards,

Paul Semmes