

# <sup>163</sup>Lu - New Formalism for the TSD4 Band

Robert Poenaru\*

September 26, 2020

Detailed report with regards to the implementation of an algorithm for finding the best parameter set which reproduces the wobbling spectrum of <sup>163</sup>Lu.

## Contents

<b>1</b>	<b>Theoretical formulation</b>	<b>1</b>
1.1	B and C terms . . . . .	2
1.2	The wobbling frequency - phonon frequency . . . . .	3
1.3	The minimum H . . . . .	3
1.4	The energy formula for the wobbling bands . . . . .	4
<b>2</b>	<b>The formalisms used in the fitting procedure</b>	<b>4</b>
2.1	Approach 1 - (A1) . . . . .	4
2.2	Approach 2 - (A2) . . . . .	6
<b>3</b>	<b>Normalization of energies: Excitation energies</b>	<b>7</b>
<b>4</b>	<b>Numerical results</b>	<b>7</b>
4.1	Experimental data set . . . . .	7
4.2	Theoretical data set - results . . . . .	8

## 1 Theoretical formulation

The formulas used in calculations involve a different number of terms which depend on the *parameter set* (the set that contains all the free parameters which need to be found).

---

\*Email: robert.poenaru@drd.unibuc.ro

## 1.1 B and C terms

These two terms enter in the expression of the *wobbling frequencies*  $\Omega_{1,2}$ . The expressions of these terms are as follows:

$$\begin{aligned}
 -B = & [(2I - 1)(A_3 - A_1) + 2jA_1] [(2I - 1)(A_2 - A_1) + 2jA_1] + 8A_2A_3I * j + \\
 & + \left( (2j - 1)(A_3 - A_1) + 2IA_1 + V \frac{2j - 1}{j(j + 1)} \sqrt{3} \left( \sqrt{3} \cos \gamma + \sin \gamma \right) \right) \cdot \\
 & \cdot \left( (2j - 1)(A_2 - A_1) + 2IA_1 + V \frac{2j - 1}{j(j + 1)} 2\sqrt{3} \sin \gamma \right) \quad (1)
 \end{aligned}$$

For  $C$ , it is convenient to break it in two sub-terms, namely:

$$\begin{aligned}
 t_C^1 = & \left[ [(2I - 1)(A_3 - A_1) + 2jA_1] \cdot \right. \\
 & \cdot \left. \left( (2j - 1)(A_3 - A_1) + 2IA_1 + V \frac{2j - 1}{j(j + 1)} \sqrt{3} \left( \sqrt{3} \cos \gamma + \sin \gamma \right) \right) - 4IjA_3^2 \right] \quad (2)
 \end{aligned}$$

and the second sub-term:

$$\begin{aligned}
 t_C^2 = & \left[ [(2I - 1)(A_2 - A_1) + 2jA_1] \cdot \right. \\
 & \cdot \left. \left( (2j - 1)(A_2 - A_1) + 2IA_1 + V \frac{2j - 1}{j(j + 1)} 2\sqrt{3} \sin \gamma \right) - 4IjA_2^2 \right] \quad (3)
 \end{aligned}$$

With these two sub-terms, final form of  $C$  is given by the straightforward calculation:

$$C = t_C^1 \cdot t_C^2 \quad (4)$$

So, when referring to the free parameters, the terms  $B$  and  $C$  are functions of the free parameters  $f = f(A_1, A_2, A_3, V, \gamma; ct)$ , where  $ct$  are just known/fixed parameters (e.g. total spin, odd-particle's a.m.).

### 1.1.1 Implementation into Mathematica

```

B[I_, j_, A1_, A2_, A3_,
  V_, \[Gamma]_] := -((2 I - 1) (A3 - A1) +
  2 j*A1)*((2 I - 1) (A2 - A1) + 2 j*A1) +
  8 A2*A3*I*
  j + ((2 j - 1) (A3 - A1) + 2 I*A1 +
  V (2 j - 1)/(j (j + 1)) Sqrt[
  3] (Sqrt[3] Cos[\[Gamma]*\[Pi]/180] +
  Sin[\[Gamma]*\[Pi]/180]))*((2 j - 1) (A2 - A1) + 2 I*A1 +
  V (2 j - 1)/(j (j + 1)) 2 Sqrt[3] Sin[\[Gamma]*\[Pi]/180]));

```

---

```

C1[I_, j_, A1_, A2_, A3_,
V_, \[Gamma]_] := (((2 I - 1) (A3 - A1) +
2 j*A1)*((2 j - 1) (A3 - A1) + 2 I*A1 +
V*(2 j - 1)/(j (j + 1)) Sqrt[
3] (Sqrt[3] Cos\[Gamma]*\[Pi]/180] +
Sin\[Gamma]*\[Pi]/180))) -
4 I*j*A3^2)*(((2 I - 1) (A2 - A1) +
2 j*A1)*((2 j - 1) (A2 - A1) + 2 I*A1 +
V*(2 j - 1)/(j (j + 1)) 2 Sqrt[3] Sin\[Gamma]*\[Pi]/180)) -
4 I*j*A2^2);

```

## 1.2 The wobbling frequency - phonon frequency

The wobbling frequency is constructed from the above mentioned terms.

$$\Omega_1 = \sqrt{\frac{1}{2} \left( -B - (B^2 - 4C)^{\frac{1}{2}} \right)} \quad (5)$$

$$\Omega_2 = \sqrt{\frac{1}{2} \left( -B + (B^2 - 4C)^{\frac{1}{2}} \right)} \quad (6)$$

**Obs:** The wobbling frequency depends on the same free parameters as  $B$  and  $C$ .

$$\Omega = f(A_1, A_2, A_3, V, \gamma)$$

### 1.2.1 Implementation into Mathematica

```

Omega1[I_, j_, A1_, A2_, A3_, V_, \[Gamma]_] := Sqrt[
1/2 (-B[I, j, A1, A2, A3,
V, \[Gamma]] - (B[I, j, A1, A2, A3, V, \[Gamma]]^2 -
4 C1[I, j, A1, A2, A3, V, \[Gamma]]^(1/2)))];

Omega2[I_, j_, A1_, A2_, A3_, V_, \[Gamma]_] := Sqrt[
1/2 (-B[I, j, A1, A2, A3,
V, \[Gamma]] + (B[I, j, A1, A2, A3, V, \[Gamma]]^2 -
4 C1[I, j, A1, A2, A3, V, \[Gamma]]^(1/2)))];

```

## 1.3 The minimum H

This term has the following expression:

$$\mathcal{H}_{\min} = (A_2 + A_3) \frac{I+j}{2} + A_1(I-j)^2 - V \frac{2j-1}{j+1} \sin\left(\gamma + \frac{\pi}{6}\right) \quad (7)$$

### 1.3.1 Implementation into Mathematica

```

HMin[I_, j_, A1_, A2_, A3_, V_, \[Gamma]_] := (A2 + A3)/2 (I + j) +
A1 (I - j)^2 -
V*(2 j - 1)/(j + 1) Sin\[Gamma]*\[Pi]/180 + \[Pi]/6];

```

---

## 1.4 The energy formula for the wobbling bands

Having the minimal  $\mathcal{H}$  term and the phonon frequencies  $\Omega$ , it is possible to express the energies of the four triaxial bands in  $^{163}\text{Lu}$  in terms of their corresponding *wobbling-phonon numbers*, namely  $n_{w_1}$  and  $n_{w_2}$ . For a given set of parameters  $A_1, A_2, A_3, V, \gamma \equiv \mathcal{P}$ , total spin  $I$ , odd-particle angular momentum  $j$  and phonon numbers, the general formula for the energy of an excited band is:

$$E_{n_{w_1}, n_{w_2}}(\mathcal{P}; I, j) = \mathcal{H}_{\min} + \Omega_1 \left( n_{w_1} + \frac{1}{2} \right) + \Omega_2 \left( n_{w_2} + \frac{1}{2} \right) \quad (8)$$

where, of course that  $\mathcal{H} = \mathcal{H}(\mathcal{P}; I, j)$  and that  $\Omega_i = \Omega_i(\mathcal{P}; I, j)$ .

### 1.4.1 Implementation into Mathematica

```
EWobb[n1_, n2_, I_, j_, A1_, A2_, A3_, V_, \[Gamma]_] :=  
  HMin[I, j, A1, A2, A3, V, \[Gamma]] +  
  Omega1[I, j, A1, A2, A3, V, \[Gamma]] (n1 + 1/2) +  
  Omega2[I, j, A1, A2, A3, V, \[Gamma]] (n2 + 1/2);
```

## 2 The formalisms used in the fitting procedure

### Experimental data and r.m.s.

When aiming at reproducing the wobbling spectrum of  $^{163}\text{Lu}$ , there are two approaches which will be used. The parameter set  $\mathcal{P}$  will be found in such a way that the root mean square error (r.m.s.) for the excited spectra of the nucleus will be the smallest possible. In both approaches, the same experimental data set will be used.

### Coupling scheme

The coupling between the even-even core and the odd-particle will also hold for both approaches, namely, in this coupling scheme, the core aligns with the  $j = 13/2$  proton.

### 2.1 Approach 1 - (A1)

In this approach, the band structure of  $^{163}\text{Lu}$  is considered to be the following:

- **TSD1:** This is the yrast band, with  $(n_{w_1}, n_{w_2}) = (0, 0)$ .
- **TSD2:**  $(n_{w_1}, n_{w_2}) = (1, 0) \rightarrow$  This is the 1-phonon excited band, built on top of TSD1 with one wobbling phonon of  $\Omega_1$  type.
- **TSD3:**  $(n_{w_1}, n_{w_2}) = (2, 0) \rightarrow$  This is 2-phonon excited band, built on top of TSD1 with two wobbling phonon excitations of  $\Omega_1$  type.

- **TSD4**: The fourth band in the wobbling spectrum of  $^{163}\text{Lu}$ . In the present calculations, it is considered to be the **chiral partner** of TSD1.

TSD4:  $(n_{w_1}, n_{w_2}) = (0, 0) \rightarrow$  ground state band, coupled to the core with the same odd-particle as the first three bands (i.e.  $j = 13/2$ ).

TSD4:  $(n_{w_1}, n_{w_2}) = (1, 0) \rightarrow$  1-phonon band, built on top of TSD1; coupled to the core with the same odd-particle as the first three bands (i.e.  $j = 13/2$ ).

### 2.1.1 Diagram with (A1) workflow

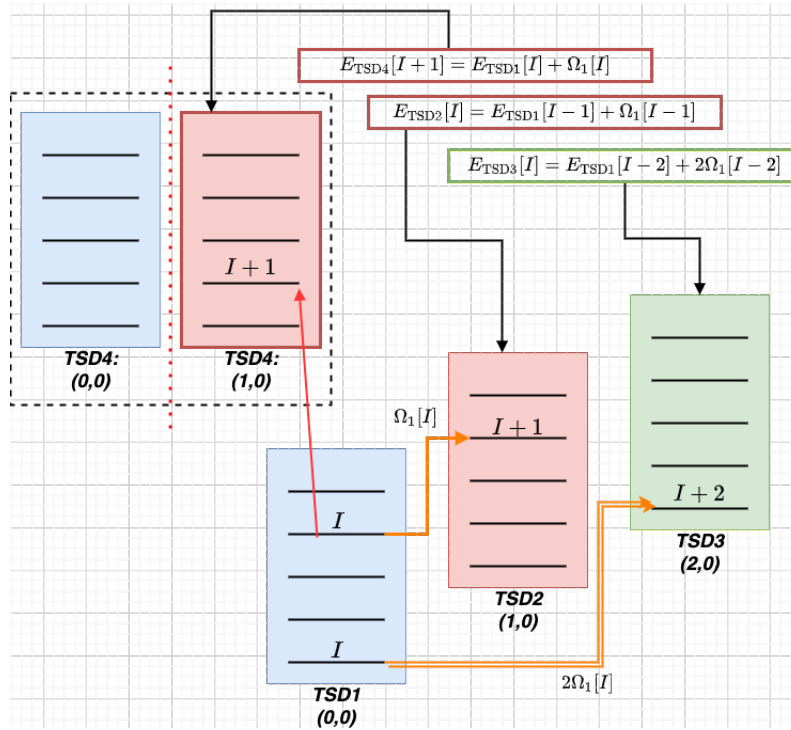


Figure 1: Workflow of (A1) approach.

### 2.1.2 Implementation into Mathematica

```
TSD1[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[0, 0, I, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

TSD2[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[1, 0, I - 1, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];
```

---

```

TSD3[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[2, 0, I - 2, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

TSD400[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[0, 0, I, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

TSD410[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[1, 0, I - 1, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

```

## 2.2 Approach 2 - (A2)

In this approach, the band structure of  $^{163}\text{Lu}$  is considered to be the following:

- **TSD1:** This is the yrast band, with  $(n_{w_1}, n_{w_2}) = (0, 0)$ .
- **TSD2:**  $(n_{w_1}, n_{w_2}) = (0, 0) \rightarrow$  Ground state band, but has a different  $R$  spin sequence than TSD1 (namely, the odd-spins  $1, 3, \dots$ ). It is considered to be the **signature partner band** of TSD1.
- **TSD3:**  $(n_{w_1}, n_{w_2}) = (1, 0) \rightarrow$  This is 1-phonon excited band, built on top of TSD2 with one wobbling phonon excitation of  $\Omega_1$  type.
- **TSD4:** The fourth band in the wobbling spectrum of  $^{163}\text{Lu}$ . In the present calculations, it is considered to be the **chiral partner** of TSD1.  
 TSD4:  $(n_{w_1}, n_{w_2}) = (0, 0) \rightarrow$  ground state band, coupled to the core with the same odd-particle as the first three bands (i.e.  $j = 13/2$ ).  
 TSD4:  $(n_{w_1}, n_{w_2}) = (1, 0) \rightarrow$  1-phonon band, built on top of TSD1; coupled to the core with the same odd-particle as the first three bands (i.e.  $j = 13/2$ ).

### 2.2.1 Implementation into Mathematica

```

TSD1[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[0, 0, I, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

TSD2[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[0, 0, I, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

TSD3[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[1, 0, I - 1, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

TSD400[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[0, 0, I, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

TSD410[I_, A1_, A2_, A3_, V_, \[Gamma]_] :=
  EWobb[1, 0, I - 1, 6.5, A1, A2, A3, V, \[Gamma]] -
  EWobb[0, 0, 6.5, 6.5, A1, A2, A3, V, \[Gamma]];

```

### 2.2.2 Diagram with (A2) workflow

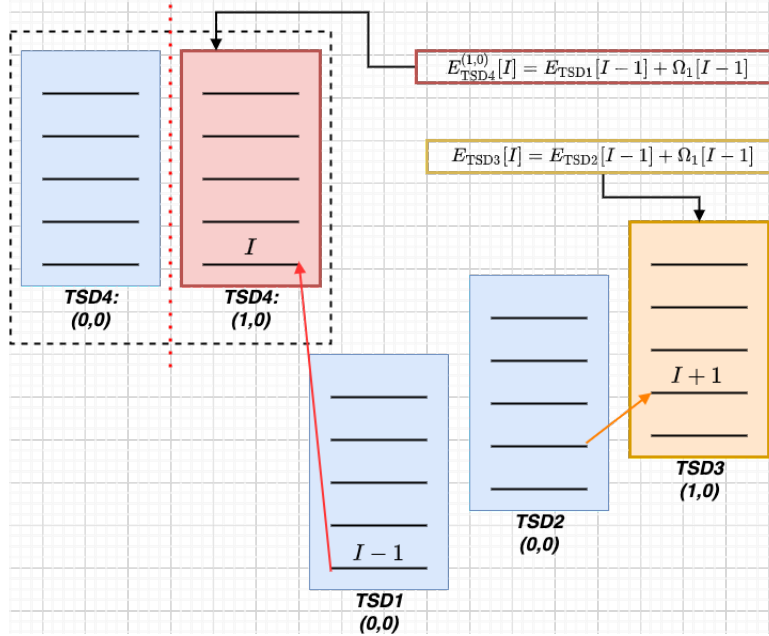


Figure 2: Workflow of (A2) approach.

## 3 Normalization of energies: Excitation energies

It is important to mention the fact that in the actual implementation of the energy expressions, the **excitation energies** were used for each band (i.e. each state  $I$  from TSD1,2,3,4 was normalized to the band-head of the yrast band. The spin of the first level of TSD1 is  $I = 13/2$ ). In Mathematica, the yrast band-head is given by:

```
EWobb[0, 0, I, 6.5, A1, A2, A3, V, \[Gamma]]
```

and this will be subtracted from each energy level.

## 4 Numerical results

### 4.1 Experimental data set

#### 4.1.1 Spins

We ignore the band head in TSD1 during calculations.

---

$I;TSD1$	$I;TSD2$	$I;TSD3$	$I;TSD4$
8.5	13.5	16.5	23.5
10.5	15.5	18.5	25.5
12.5	17.5	20.5	27.5
14.5	19.5	22.5	29.5
16.5	21.5	24.5	31.5
18.5	23.5	26.5	33.5
20.5	25.5	28.5	35.5
22.5	27.5	30.5	37.5
24.5	29.5	32.5	39.5
26.5	31.5	34.5	41.5
28.5	33.5	36.5	
30.5	35.5	38.5	
32.5	37.5	40.5	
34.5	39.5	42.5	
36.5	41.5		
38.5	43.5		
40.5	45.5		
42.5			
44.5			
46.5			
48.5			

Table 1: The spin values  $I$  for all the wobbling bands of  $^{163}\text{Lu}$ .

#### 4.1.2 Energies

We ignore the band head in TSD1 during calculations.

## 4.2 Theoretical data set - results

The energies below are all evaluated at a given parameter set  $\mathcal{P}$ , which is determined from the **fitting procedure**. The procedure is searching through all the intervals (established before the search function) for  $A_k$ ,  $V$  and  $\gamma$  and trying to find the most optimal combination that minimize the deviations from the experimental values of the excitation energies.

Essentially, the only difference between (A1) and (A2) exists in the TSD2 and TSD3 bands, since they differ in the wobbling phonon excitation numbers. The excitation energies for TSD4 (namely, both TSD4(0,0) and (1,0) will be identical across both approaches).



---

$I$	$E_{\text{exc}}; TSD1$
8.5	0.1966
10.5	0.4597
12.5	0.7746
14.5	1.1609
16.5	1.6112
18.5	2.1265
20.5	2.7051
22.5	3.3441
24.5	4.0411
26.5	4.7937
28.5	5.5992
30.5	6.457
32.5	7.3667
34.5	8.3293
36.5	9.3458
38.5	10.4169
40.5	11.5431
42.5	12.7224
44.5	13.9491
46.5	15.2181
48.5	16.5221

Table 2: Experimental excitation energies of TSD1.

#### 4.2.1 Fit parameters

The fit parameters are obtained from a C++ implementation, and the results are as follows:

- $\mathcal{I}_1 = 77$
- $\mathcal{I}_2 = 47$
- $\mathcal{I}_3 = 3$
- $V = 2.1$
- $\gamma = 16$

With the coupling odd particle's a.m.  $j = 13/2$ . This is the parameter set, further denoted by  $\mathcal{P}$ .

---

$I$	$E_{\text{exc}}; TSD2$
13.5	1.3394
15.5	1.7467
17.5	2.2184
19.5	2.7527
21.5	3.3484
23.5	4.003
25.5	4.7143
27.5	5.4805
29.5	6.3004
31.5	7.1733
33.5	8.0998
35.5	9.08
37.5	10.1147
39.5	11.2036
41.5	12.3466
43.5	13.5441
45.5	14.7911

Table 3: Experimental excitation energies of TSD2.

$I$	$E_{\text{exc}}; TSD3$
13.5	1.3394
15.5	1.7467
17.5	2.2184
19.5	2.7527
21.5	3.3484
23.5	4.003
25.5	4.7143
27.5	5.4805
29.5	6.3004
31.5	7.1733
33.5	8.0998
35.5	9.08
37.5	10.1147
39.5	11.2036
41.5	12.3466
43.5	13.5441
45.5	14.7911

Table 4: Experimental excitation energies of TSD3.

---

$I$	$E_{\text{exc}}; TSD4$
23.5	4.58
25.5	5.2251
27.5	5.9273
29.5	6.6819
31.5	7.4919
33.5	8.3573
35.5	9.2778
37.5	10.2535
39.5	11.2851
41.5	12.3701

Table 5: Experimental excitation energies of TSD4.

$I$	$B$	$C$	$\mathcal{H}$	$\Omega_1$	$\Omega_2$	$E_{\text{exc}}; TSD1$
8.5	-3.64714	0.282392	-1.06122	0.281329	1.88891	0.279046
10.5	-4.09819	0.405594	-0.805993	0.318562	1.99918	0.608022
12.5	-4.57184	0.556663	-0.498818	0.353818	2.10871	0.987591
14.5	-5.06808	0.739429	-0.139695	0.387763	2.21759	1.41813
16.5	-5.58692	0.957894	0.271376	0.42079	2.32591	1.89987
18.5	-6.12835	1.21623	0.734395	0.453145	2.43372	2.43298
20.5	-6.69237	1.51879	1.24936	0.484984	2.54109	3.01755
22.5	-7.27899	1.87008	1.81628	0.516415	2.64808	3.65367
24.5	-7.8882	2.27479	2.43514	0.547514	2.75471	4.3414
26.5	-8.52	2.73779	3.10595	0.578332	2.86104	5.08078
28.5	-9.1744	3.26412	3.82871	0.608909	2.96709	5.87186
30.5	-9.85139	3.85897	4.60342	0.639274	3.0729	6.71465
32.5	-10.551	4.52772	5.43008	0.669451	3.17849	7.60919
34.5	-11.2732	5.27593	6.30868	0.699458	3.28389	8.5555
36.5	-12.0179	6.10932	7.23923	0.729308	3.38911	9.55358
38.5	-12.7853	7.03377	8.22173	0.759016	3.49416	10.6035
40.5	-13.5753	8.05536	9.25618	0.788589	3.59908	11.7052
42.5	-14.3878	9.18032	10.3426	0.818038	3.70387	12.8587
44.5	-15.223	10.4151	11.4809	0.84737	3.80853	14.064
46.5	-16.0807	11.7662	12.6712	0.876592	3.91309	15.3212
48.5	-16.961	13.2404	13.9135	0.90571	4.01755	16.6302

Table 6: Approach (A1) - Theoretical values for TSD1, evaluated for the parameter set  $\mathcal{P}$  given in text.

---

$I$	$B$	$C$	$\mathcal{H}$	$\Omega_1$	$\Omega_2$	$E_{\text{exc}}; TSD2$
13.5	-4.81714	0.643838	-0.32575	0.370925	2.16323	1.34141
15.5	-5.32468	0.843942	0.0593469	0.404374	2.27182	1.80589
17.5	-5.85481	1.08181	0.496392	0.43704	2.37987	2.32066
19.5	-6.40754	1.3617	0.985385	0.469121	2.48746	2.88612
21.5	-6.98286	1.68805	1.52633	0.500745	2.59463	3.50253
23.5	-7.58077	2.06546	2.11922	0.532003	2.70143	4.17008
25.5	-8.20128	2.4987	2.76405	0.562955	2.80791	4.88891
27.5	-8.84438	2.99272	3.46084	0.593648	2.9141	5.65911
29.5	-9.51007	3.55265	4.20957	0.624116	3.02002	6.48077
31.5	-10.1984	4.18377	5.01025	0.654385	3.12572	7.35393
33.5	-10.9092	4.89154	5.86288	0.684475	3.23121	8.27864
35.5	-11.6427	5.68161	6.76746	0.714402	3.33652	9.25496
37.5	-12.3988	6.55978	7.72399	0.744179	3.44165	10.2829
39.5	-13.1774	7.53204	8.73246	0.773819	3.54664	11.3625
41.5	-13.9787	8.60452	9.79288	0.803329	3.65149	12.4937
43.5	-14.8026	9.78356	10.9053	0.832719	3.75621	13.6767
45.5	-15.649	11.0757	12.0696	0.861995	3.86082	14.9114

Table 7: Approach (A1) - Theoretical values for TSD2, evaluated for the parameter set  $\mathcal{P}$  given in text.

$I$	$B$	$C$	$\mathcal{H}$	$\Omega_1$	$\Omega_2$	$E_{\text{exc}}; TSD3$
16.5	-5.58692	0.957894	0.271376	0.42079	2.32591	2.19366
18.5	-6.12835	1.21623	0.734395	0.453145	2.43372	2.74145
20.5	-6.69237	1.51879	1.24936	0.484984	2.54109	3.33926
22.5	-7.27899	1.87008	1.81628	0.516415	2.64808	3.98752
24.5	-7.8882	2.27479	2.43514	0.547514	2.75471	4.6865
26.5	-8.52	2.73779	3.10595	0.578332	2.86104	5.43643
28.5	-9.1744	3.26412	3.82871	0.608909	2.96709	6.23745
30.5	-9.85139	3.85897	4.60342	0.639274	3.0729	7.08968
32.5	-10.551	4.52772	5.43008	0.669451	3.17849	7.9932
34.5	-11.2732	5.27593	6.30868	0.699458	3.28389	8.9481
36.5	-12.0179	6.10932	7.23923	0.729308	3.38911	9.95441
38.5	-12.7853	7.03377	8.22173	0.759016	3.49416	11.0122
40.5	-13.5753	8.05536	9.25618	0.788589	3.59908	12.1215
42.5	-14.3878	9.18032	10.3426	0.818038	3.70387	13.2823

Table 8: Approach (A1) - Theoretical values for TSD3, evaluated for the parameter set  $\mathcal{P}$  given in text.

---

$I$	$B$	$C$	$\mathcal{H}$	$\Omega_1$	$\Omega_2$	$E_{\text{exc}}; TSD4(0, 0)$
23.5	-7.58077	2.06546	2.11922	0.532003	2.70143	3.99108
25.5	-8.20128	2.4987	2.76405	0.562955	2.80791	4.70463
27.5	-8.84438	2.99272	3.46084	0.593648	2.9141	5.46986
29.5	-9.51007	3.55265	4.20957	0.624116	3.02002	6.28679
31.5	-10.1984	4.18377	5.01025	0.654385	3.12572	7.15545
33.5	-10.9092	4.89154	5.86288	0.684475	3.23121	8.07587
35.5	-11.6427	5.68161	6.76746	0.714402	3.33652	9.04807
37.5	-12.3988	6.55978	7.72399	0.744179	3.44165	10.072
39.5	-13.1774	7.53204	8.73246	0.773819	3.54664	11.1478
41.5	-13.9787	8.60452	9.79288	0.803329	3.65149	12.2754

Table 9: Approach (A1) - Theoretical values for TSD4(0,0), evaluated for the parameter set  $\mathcal{P}$  given in text.

$I$	$E_{\text{exc}}; TSD4(0, 0)$	$E_{\text{exc}}; TSD4(1, 0)$
23.5	3.99108	4.17008
25.5	4.70463	4.88891
27.5	5.46986	5.65911
29.5	6.28679	6.48077
31.5	7.15545	7.35393
33.5	8.07587	8.27864
35.5	9.04807	9.25496
37.5	10.072	10.2829
39.5	11.1478	11.3625
41.5	12.2754	12.4937

Table 10: Approach (A1) - Theoretical excitation energies (only) values for TSD4(0,0) and TSD4(1,0), evaluated for the parameter set  $\mathcal{P}$  given in text.

---

$I$	$B$	$C$	$\mathcal{H}$	$\Omega_1$	$\Omega_2$	$E_{\text{exc}}; TSD2$
13.5	-4.81714	0.643838	-0.32575	0.370925	2.16323	1.19647
15.5	-5.32468	0.843942	0.0593469	0.404374	2.27182	1.65259
17.5	-5.85481	1.08181	0.496392	0.43704	2.37987	2.16
19.5	-6.40754	1.3617	0.985385	0.469121	2.48746	2.71882
21.5	-6.98286	1.68805	1.52633	0.500745	2.59463	3.32916
23.5	-7.58077	2.06546	2.11922	0.532003	2.70143	3.99108
25.5	-8.20128	2.4987	2.76405	0.562955	2.80791	4.70463
27.5	-8.84438	2.99272	3.46084	0.593648	2.9141	5.46986
29.5	-9.51007	3.55265	4.20957	0.624116	3.02002	6.28679
31.5	-10.1984	4.18377	5.01025	0.654385	3.12572	7.15545
33.5	-10.9092	4.89154	5.86288	0.684475	3.23121	8.07587
35.5	-11.6427	5.68161	6.76746	0.714402	3.33652	9.04807
37.5	-12.3988	6.55978	7.72399	0.744179	3.44165	10.072
39.5	-13.1774	7.53204	8.73246	0.773819	3.54664	11.1478
41.5	-13.9787	8.60452	9.79288	0.803329	3.65149	12.2754
43.5	-14.8026	9.78356	10.9053	0.832719	3.75621	13.4549
45.5	-15.649	11.0757	12.0696	0.861995	3.86082	14.6861

Table 11: Approach (A2) - Theoretical values for TSD2, evaluated for the parameter set  $\mathcal{P}$  given in text.

$I$	$B$	$C$	$\mathcal{H}$	$\Omega_1$	$\Omega_2$	$E_{\text{exc}}; TSD3$
16.5	-5.58692	0.957894	0.271376	0.42079	2.32591	2.05696
18.5	-6.12835	1.21623	0.734395	0.453145	2.43372	2.59704
20.5	-6.69237	1.51879	1.24936	0.484984	2.54109	3.18794
22.5	-7.27899	1.87008	1.81628	0.516415	2.64808	3.82991
24.5	-7.8882	2.27479	2.43514	0.547514	2.75471	4.52308
26.5	-8.52	2.73779	3.10595	0.578332	2.86104	5.26759
28.5	-9.1744	3.26412	3.82871	0.608909	2.96709	6.06351
30.5	-9.85139	3.85897	4.60342	0.639274	3.0729	6.91091
32.5	-10.551	4.52772	5.43008	0.669451	3.17849	7.80984
34.5	-11.2732	5.27593	6.30868	0.699458	3.28389	8.76035
36.5	-12.0179	6.10932	7.23923	0.729308	3.38911	9.76247
38.5	-12.7853	7.03377	8.22173	0.759016	3.49416	10.8162
40.5	-13.5753	8.05536	9.25618	0.788589	3.59908	11.9217
42.5	-14.3878	9.18032	10.3426	0.818038	3.70387	13.0788

Table 12: Approach (A2) - Theoretical values for TSD3, evaluated for the parameter set  $\mathcal{P}$  given in text.