Symmetry analysis of trimers rovibrational spectra: the case of Ne_3

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Abstract. An approximate method to assign the symmetry to the rovibrational spectrum of homonuclear treatments based on the solution of the rotational Hamiltonian by means of a purely vibrational basis combined with standard rotational functions is applied on Ne_3 . The neon trimer constitutes an ideal test between heavier systems such as Ar_3 for which the method proves to be an extremely useful technique and some other previously investigated cases such as H_3^+ where some limitations were observed. Comparisons of the calculated rovibrational energy levels are established with results from different calculations reported in the literature.

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1 Introduction

Rare gas (RG) trimers have been the subject of a large list of works focussed in the study of their bound states energies and structures [1–10]. Theoretical approaches developed to characterize the molecular rotation-vibration structure have been currently tested on these kind of systems [11–16]. Among all these numerous investigations we proposed some time ago a method to calculate and assign the corresponding symmetry character to the rovibrational spectra of Ar_3 for different values of the total angular momentum $J > 0$ [17, 18]. The approach was based in a previously developed method to solve the pure vibrational problem, $J = 0$, using a basis set constructed with distributed Gaussian functions (DGFs) on the interparticle distances [19]. This method for the rotationless case was successfully applied for different RG trimers [20–23], and subsequently extended to treat $J > 0$ situations [24–26]. In the same spirit of a comparative analysis performed before between different RG trimers [5, 21] we test in this work the DGF rotation-vibration approach developed in Ref. [17] with Ne_3 . The difference with mass in comparison with the Ar trimer, an example for which the performance of the presently discussed method was found remarkably good [17, 18], is expected to constitute a more demanding challenge. In fact, a previous application [27] on a much lighter system such as H_3^+ revealed some limitations due to the importance of the contribution from

Coriolis distortion terms which the present approximative approach does not explicitly account for.

The rotational spectrum of Ne_3 has been investigated before by different authors. For example, Salci *et al.* [13] employed a finite elements method (FEM) to calculate rovibrational states up to $J = 3$ assuming the trimer as an oblate symmetric top. The comparison with the analytical expression of the energy levels corresponding to a symmetric planar trimer revealed increasing differences with the vibrational excitation. Moreover significant contribution from Coriolis coupling terms was observed. The hyperspherical coordinates (HC) calculation by Suno *et al.* [15] employed the same pairwise potential than Ref. [13] and reported results up to $J = 6$. Finally, energy levels and wave functions corresponding to the neon trimer bound states were obtained in quantum dynamical calculations by Yang *et al.* [14] between $J = 0 - 18$ using a Lennard-Jones potential. In this work we compare with some of these most recent studies on the title system to test the capabilities of the DGF method to treat the rotation-vibration spectrum of these RG trimers.

The paper is structured as follows: Theoretical details of the DGF method are given in Section 2; results are discussed in Section 3 with a separate comparison with results from Refs. [13] and [15], and finally, conclusions are shown in Section 4.

2 Theory

The method proposed in previous investigations of Ar₃ [17,18] assumes the total Hamiltonian as the sum of a vibrational and a rotational part: $H_T = H_V + H_R$. The expression of H_V in terms of interparticle distances R_i for the case of three identical atoms with mass m_i , can be finally expressed, after transformations of the total wave function [20,24], as follows:

$$H_V = \sum_{i=1}^3 \left\{ \frac{-\hbar^2}{m_i} \left[\frac{\partial^2}{\partial R_i^2} + \frac{1}{R_i} + \frac{\partial}{\partial R_i} - \frac{1}{4R_i^2} + T_{ijk} \right] \right\} + U(\mathbf{R}) \quad (1)$$

where $U(\mathbf{R})$ is the potential energy operator and the T_{ijk} operator, with $i \neq j \neq k$, is written as:

$$T_{ijk} = \cos\theta_i \left[\nabla_j \nabla_k - \frac{\nabla_k}{2R_j} - \frac{\nabla_j}{2R_k} + \frac{1}{4R_j R_k} \right] \quad (2)$$

where $\nabla_i = \partial/\partial R_i$ and

$$\cos\theta_i = \frac{R_j^2 + R_k^2 - R_i^2}{2R_j R_k} \quad (3)$$

For H_R , we choose the case of an asymmetric top [28–30]:

$$H_R = \frac{1}{2}(A + C)\mathbf{J}^2 + \frac{1}{2}(A - C)(J_A^2 + \kappa J_B^2 - J_C^2) \quad (4)$$

where $\kappa = (2B - A - C)/(A - C)$ is Ray's asymmetry parameter [31] and A , B and C are rotational constants.

In order to solve the vibrational part, we employ symmetry adapted basis functions for each irreducible representation corresponding to the C_{3v} group for homonuclear trimers as follows:

$$\begin{aligned} \phi_j(\mathbf{R}) = & \frac{1}{\sqrt{6}} \{ \chi(E) \mathcal{G}_{lmn}^{123}(\mathbf{R}) + \chi(C_3) [\mathcal{G}_{lmn}^{231}(\mathbf{R}) + \mathcal{G}_{lmn}^{312}(\mathbf{R})] \\ & + \chi(\sigma_v) [\mathcal{G}_{lmn}^{213}(\mathbf{R}) + \mathcal{G}_{lmn}^{132}(\mathbf{R}) + \mathcal{G}_{lmn}^{321}(\mathbf{R})] \} \end{aligned} \quad (5)$$

where the $\mathcal{G}_{lmn}^{123}(\mathbf{R})$ are products of $\varphi_p(R_i)$ Gaussian functions for the R_i distance with center at the value R_p :

$$\mathcal{G}_{lmn}^{123}(\mathbf{R}) = \varphi_l(R_1) \varphi_m(R_2) \varphi_n(R_3) \quad (6)$$

$\chi(E)$, $\chi(C_3)$ and $\chi(\sigma_v)$ are the characters for the C_{3v} group, and once their corresponding values are introduced in Equation (5) for each irreducible representation, we obtain the following basis functions set for A_1 , A_2 and E as follows:

$$\begin{aligned} \phi_j^{A_1}(\mathbf{R}) = & \frac{1}{\sqrt{6}} [\mathcal{G}_{lmn}^{123}(\mathbf{R}) + \mathcal{G}_{lmn}^{231}(\mathbf{R}) + \mathcal{G}_{lmn}^{312}(\mathbf{R}) \\ & + \mathcal{G}_{lmn}^{213}(\mathbf{R}) + \mathcal{G}_{lmn}^{132}(\mathbf{R}) + \mathcal{G}_{lmn}^{321}(\mathbf{R})] \end{aligned} \quad (7)$$

$$\begin{aligned} \phi_j^{A_2}(\mathbf{R}) = & \frac{1}{\sqrt{6}} [\mathcal{G}_{lmn}^{123}(\mathbf{R}) + \mathcal{G}_{lmn}^{231}(\mathbf{R}) + \mathcal{G}_{lmn}^{312}(\mathbf{R}) \\ & - \mathcal{G}_{lmn}^{213}(\mathbf{R}) - \mathcal{G}_{lmn}^{132}(\mathbf{R}) - \mathcal{G}_{lmn}^{321}(\mathbf{R})] \end{aligned} \quad (8)$$

$$\phi_j^E(\mathbf{R}) = \frac{1}{\sqrt{6}} [2\mathcal{G}_{lmn}^{123}(\mathbf{R}) - \mathcal{G}_{lmn}^{231}(\mathbf{R}) - \mathcal{G}_{lmn}^{312}(\mathbf{R})] \quad (9)$$

In combination with the eigenfunctions of H_V for the $J = 0$ case, we construct a basis set employing standard rotational basis functions in terms of J and its projections on the z axis of the body-fixed (Ω) and space-fixed (M) frames to diagonalize H_R from Equation (4). As a result of the above discussed approach to obtain the rovibrational spectrum, the symmetry of the total wave function for the corresponding bound states can be expressed as the product:

$$\Gamma = \Gamma_V^{\Omega\ell} \times \Gamma_R \quad (10)$$

where Γ_R refers to the symmetry of the strictly rotational part, while $\Gamma_V^{\Omega\ell}$ refers to a rovibrational part, where ℓ is the vibrational angular momentum number [28]. In our previous studies [17,18] we developed a recipe to assign the character for Γ_R and $\Gamma_V^{\Omega\ell}$. In essence we can summarize as follows: If $\Omega = 0$, $\Gamma_R = A_1$ (A_2) for even (odd) values of J , and $\Gamma_R = A_1$ or A_2 for $\Omega \neq 0$. On the other hand, for the rovibrational part, if we define $\eta = |\pm 2\ell - \Omega|$, with $\ell, \Omega \geq 0$, the rule consists on: (i) $\Gamma_V^{\Omega\ell} = A_1$ for $\eta = 0$; (ii) $\Gamma_V^{\Omega\ell} = A_1, A_2$ for η multiple of 3; and (iii) $\Gamma_V^{\Omega\ell} = E$ if η is not multiple of 3. Finally, and due to the fact that our basis set has been adapted to symmetry according to the C_{3v} group instead of D_{3h} , the total symmetry Γ in equation (10) is ' or ' ' depending on whether Ω is even or odd, respectively.

In order to assign the quantum number ℓ to the vibrational states obtained with the DGF approach, the HC method from Ref. [18] has been used. The DGF calculation was performed using up to 50 Gaussian functions $\varphi_i(R)$ with centers starting from 2.38 Å equally spaced with an interval of 0.16 Å. A total number of 19,053 $\phi_j^{A_1}$ functions from Equation (7) were generated for the A_1 representation; 15,877 $\phi_j^{A_2}$ functions from Equation (8) for the representation A_2 and, finally 36,790 ϕ_j^E functions from Equation (9) for E . Details of how the matrix elements of the total Hamiltonian, which contains crossed terms between Ω and $\Omega \pm 2$, and are calculated in a DGF basis set have been given before and the interested reader is referred to those previous papers [24,17,18]. For the scope of this work, it will suffice by indicating that the integration in each R_i coordinate involved in both H_V and H_R of Equations (1) and (4), respectively, is solved applying a mean-value approach for the centers of the DGF.

In this work present DGF results have been compared with those reported from the previous investigations on Ne₃ by Salci *et al.* [13] and by Suno [15]. The potential energy operator $U(\mathbf{R})$ in Equation (1) employed in the calculations was the HFD-B pairwise potential by Aziz and Slaman [32].

3 Results

3.1 Comparison with calculation by Salci *et al.* [13]

The calculation by means of the FEM method by Salci *et al.* [13], as opposed to the study performed by Suno [15]

Table 1. Energy levels of the Ne₃ rovibrational states for $J = 0$ (in cm⁻¹) obtained in this work by means of HC (third column) and DGF (seventh column) methods. The ℓ number is given in the second column and the v^Γ vibrational number for each irreducible representation is in the sixth column. Energies and the v number for the vibrational states from Ref. [13] are given in the fourth and fifth columns, respectively.

HC			FEM [13]		DGF	
Γ	ℓ	E	v	E	v^Γ	E_{DGF}
A'_1	0	-51.51	0	-51.50	1	-51.51
	0	-36.44	2	-36.43	2	-36.44
	3	-34.22	4	-34.22	3	-34.35
	0	-31.64	6	-31.63	4	-31.85
	0	-28.04	8	-28.04	5	-28.22
	0	-24.09	10	-24.08	6	-24.14
	0	-22.46	12	-22.45	7	-22.46
	0	-21.91	14	-21.90	8	-22.06
	0	-19.22	18	-19.21	9	-19.17
E'	1	-38.76	1	-38.75	1	-38.76
	1	-34.63	3	-34.63	2	-34.71
	2	-32.42	5	-32.42	3	-32.63
	2	-28.65	7	-28.64	4	-28.87
	1	-24.55	9	-24.54	5	-24.57
	1	-23.46	11	-23.45	6	-23.48
	1	-22.36	13	-22.34	7	-22.44
	1	-20.23	15	-20.23	8	-20.26
	1	-19.65	17	-19.65	9	-19.62
A'_2	3	-20.06	16	-20.05	1	-20.06
	3	-18.50	19	-18.49	2	-18.60

focussed only in the A'_1 and A'_2 levels, comprised three different irreducible representations (A'_1 , A'_2 and E'). We will therefore use the comparison with the former results to detail some of the aspects of the symmetry assignment procedure of the DGF method.

One of the first steps consists on the assignment of the ℓ number to the H_V eigenstates obtained with the DGF approach required for the symmetry characterization of the rotational spectra. This is usually achieved by simply comparison for the $J = 0$ energy levels with the results obtained by means of a HC calculation. Table 1 shows vibrational levels obtained in this work with HC and DGF methods in comparison with results reported in Ref. [13]. The energy values of the A'_1 levels from Ref. [18] are in perfect agreement with the present HC calculation, which extends, as shown in Table 1, to the E' and A'_2 groups. The diagonalization of the rotationless Hamiltonian of Equation (1) in separate symmetry-adapted basis functions as shown in Equations (7)-(9) reveals that even values of the index v in the work by Salci *et al.* [13] corresponds to the A'_1 representation whereas odd values are for the E' block. The only exception to this were the lowest states of the A'_2 irreducible representation which appears below ~ -20 cm⁻¹. On the other hand the A'_1 block is the only one containing states with $\ell = 0$.

Table 2. Comparison between energy levels of the Ne₃ rovibrational states for $J = 1$, measured in cm⁻¹ obtained by means of the FEM method of Ref. [13] (third column) and the present DGF (ninth column).

Γ_{FEM}	Ω	E_{FEM}	$\Gamma_V^{\Omega\ell}$	Γ_R	Γ	v^Γ	ℓ	E_{DGF}
A	0	-51.18	A_1	A_2	A'_2	1^{A_1}	0	-51.19
	1	-38.49	A_1/A_2	A_1/A_2	A'_2	1^E	1	-38.52
	1	-38.40	A_1/A_2	A_1/A_2	A'_1	1^E	1	-38.50
	0	-36.08	A_1	A_2	A'_2	2^{A_1}	0	-36.08
E	1	-51.26	E	A_1/A_2	E''	1^{A_1}	0	-51.27
	1	-38.59	E	A_1/A_2	E''	1^E	1	-38.55
	0	-38.43	E	A_2	E'	1^E	1	-38.45
	1	-36.19	E	A_2	E''	2^{A_1}	0	-36.18

The comparison between the rovibrational states for $J = 1$ obtained with the present DGF method and those reported in the FEM calculation [13] is shown in Table 2. The assignment of the symmetry allows a more detailed characterization into the different irreducible representation blocks. The ground vibrational 1^E is found to be responsible of states in each of these symmetry groups E , A_1 and A_2 , with the ' and ' ' character depending on the even/odd Ω . In view of the restricted energy range considered by Salci *et al.* in their work, none of the $J = 0$ levels from the A'_2 group shown in Table 1 contributes to the $J = 1$ spectrum considered in this calculation. In turn, both 1^{A_1} and 2^{A_1} vibrational states are responsible of, respectively, the ground and first excited $J = 1$ levels of A'_2 and E'' . The agreement between the DGF and FEM calculations for the energy values is remarkable, thus suggesting the good capabilities of the former approach, at least for these low energy levels of the $J > 0$ case.

A similar impression is obtained when the calculation extends to $J = 3$. The comparison between results from the DGF approach and the FEM study reported in Ref. [13] shown in Table 3 reveals differences between the corresponding energy values which do not exceed ~ 0.2 cm⁻¹ in any case. Ground states in every irreducible representation come from the 1^{A_1} vibrational state from the $J = 0$ calculation, with degenerate levels which separate between A'_1 and A'_2 . The larger number of different possibilities for Ω makes the $J = 3$ spectrum denser although, as discussed before for the $J = 1$ case, the only vibrational states involved are 1^{A_1} , 2^{A_1} and 1^E . As shown in Table 3 the symmetry of all states from the E group mainly comes from the rovibrational part. In all cases, the η number (see Section 2) becomes non multiple of 3 and, therefore $\Gamma_V^{\Omega\ell} = E$, a feature which solves the uncertainty between A_1 and A_2 coming from the rotational part Γ_R .

3.2 Comparison with calculation by Suno [15]

The rovibrational states obtained in Ref. [15] corresponds exclusively to the A group and the only distinction is considered as a function of the even/odd character of Ω , thus

Table 3. Same as Table 2 for $J = 3$.

Γ	Ω	E_{FEM}	$\Gamma_V^{\Omega\ell}$	Γ_R	Γ	v^Γ	ℓ	E_{DGF}
A	3	-50.33	A_1/A_2	A_1/A_2	A_1''	1^{A_1}	0	-50.35
	3	-50.33	A_1/A_2	A_1/A_2	A_2''	1^{A_1}	0	-50.35
	0	-49.61	A_1	A_2	A_2'	1^{A_1}	0	-49.62
	2	-37.44	A_1	A_1/A_2	A_1'	1^E	1	-37.44
	2	-37.39	A_1	A_1/A_2	A_1''	1^E	1	-37.29
	1	-37.20	A_1/A_2	A_1/A_2	A_1''	1^E	1	-37.21
	1	-36.67	A_1/A_2	A_1/A_2	A_2''	1^E	1	-36.81
	3	-35.38	A_1/A_2	A_1/A_2	A_1''	2^{A_1}	0	-35.29
	0	-34.53	A_1	A_2	A_2'	2^{A_1}	0	-34.35
E	2	-49.93	E	A_1/A_2	E'	1^{A_1}	0	-49.94
	1	-49.69	E	A_1/A_2	E''	1^{A_1}	0	-49.70
	3	-37.91	E	A_1/A_2	E''	1^E	1	-37.65
	3	-37.53	E	A_1/A_2	E''	1^E	1	-37.63
	2	-37.27	E	A_1/A_2	E'	1^E	1	-37.25
	1	-37.02	E	A_1/A_2	E''	1^E	1	-37.01
	0	-36.75	E	A_1/A_2	E'	1^E	1	-36.85
	2	-34.86	E	A_1/A_2	E'	2^{A_1}	0	-34.84
	1	-34.66	E	A_1/A_2	E''	2^{A_1}	0	-34.58

Table 4. Comparison between energy levels of the Ne₃ rovibrational states for $J = 1$, measured in cm⁻¹ obtained in Ref. [15] (second column) and the present DGF calculation (seventh column).

v	E [15]	Γ	Ω	v^Γ	ℓ	E_{DGF}
0 ⁻	-38.42	A_1''	1	1^E	1	-38.50
1 ⁻	-33.70		1	2^E	1	-33.83
2 ⁻	-30.60		1	3^E	1	-31.14
3 ⁻	-26.33		1	4^E	1	-27.35
4 ⁻	-24.12		1	5^E	1	-24.13
5 ⁻	-21.05		1	6^E	1	-22.16
6 ⁻	-20.86		1	7^E	1	-21.16
7 ⁻	-19.64		1	8^E	1	-19.42
8 ⁻	-18.64		1	9^E	1	-18.69
0 ⁺	-19.69	A_1'	0	1^{A_2}	3	-19.72
1 ⁺	-17.50		0	2^{A_2}	3	-17.35

leading to the A_1'' and A_1' cases respectively. In Reference [15] levels have been identified as $v^\pm$ to distinguish between both groups. Once the assignment of the ℓ number to the DGF states for $J = 0$ has already been made before (see Table 1) we start directly with $J = 1$. The comparison between present results and those obtained in the calculation by Suno directly for that value of the total angular momentum is shown in Table 4. The $J = 1$ spectrum, restricted in this case to the A group, involves more vibrational states than the previous comparison with results by Salci *et al.* [13]. In particular, all the $J = 0$ spectrum corresponding to the E block shown in Table 1 for the rotationless case, is present as original seeds of the rovibrational levels of the A_1'' group in Table 4. The accord

Table 5. Same as Table 4 for $J = 4$.

v	E [15]	Γ	Ω	v^Γ	ℓ	E_{DGF}
0 ⁻	-49.08	A_1''	3	1^{A_1}	0	-49.09
1 ⁻	-36.22		1	1^E	1	-35.70
2 ⁻	-34.09		3	2^{A_1}	0	-34.09
3 ⁻	-32.24		1	2^E	1	-32.23
4 ⁻	-29.69		3	3^{A_1}	3	-30.00
5 ⁻	-28.86		1	3^E	1	-29.45
6 ⁻	-25.22		3	5^E	0	-25.15
0 ⁺	-48.36	A_1'	0	1^{A_1}	0	-48.37
1 ⁺	-36.90		4	1^E	1	-36.97
2 ⁺	-36.21		2	1^E	1	-36.04
3 ⁺	-33.73		0	2^{A_1}	0	-34.04
4 ⁺	-33.10		4	2^E	1	-31.83
5 ⁺	-31.40		4	2^E	1	-31.30
6 ⁺	-30.83		2	3^E	1	-30.23
7 ⁺	-28.11		0	3^{A_1}	3	-28.15

between the values of the energies is also good although slightly larger differences are seen than in the comparison established in Table 2 with results from Ref. [13]. The onset of the A_1' branch, on the other hand, occurs at much higher energies, in fact the ground state of such symmetry block lies above seven states of A_1'' , although in the calculation by Suno [15] the energy difference between such a A_1' ground state and the 7⁻ state of the A_1'' block is smaller than the difference found in our study.

Calculations for larger values of the total angular momentum have been performed using the DGF approach. The comparison with results obtained in the work by Suno [15] for $J = 4$ and 5 is presented in Tables 5 and 6, respectively. The agreement between both set of energies is certainly good for almost the entire spectrum under consideration. The increase in the values of Ω as J becomes larger does not constitute, for the symmetry blocks here investigated, any difficulty for the method.

Although we do not show it here (a different potential energy surface and even mass for the Ne atom are considered with respect to the previously discussed calculations) the comparison with values reported in a similar investigation of the Ne trimer rotational spectrum by Yang [14] also support the validity of the present DGF method. In fact, despite the lighter mass, Ne₃ constitutes, as Ar₃ [17,18], a good test to prove the capabilities of the approach both to calculate the rovibrational states of molecular trimers and to characterize the symmetry of such levels.

4 Conclusions

A previously proposed method based in the use of distributed Gaussian functions (DGF) to calculate and characterize the rovibrational spectrum of trimers has been employed for the case of Ne₃. The comparison with previous investigations of the spectra for this system has revealed that the DGF method allows the calculation of the

Table 6. Same as Table 5 for $J = 5$.

v	E [15]	Γ	Ω	v^Γ	ℓ	E_{DGF}
0 ⁻	-47.52	A_1''	3	1 ^{A₁}	0	-47.52
1 ⁻	-36.73		5	1 ^E	1	-36.17
2 ⁻	-33.81		1	1 ^E	1	-33.77
3 ⁻	-32.60		3	2 ^{A₁}	0	-32.63
4 ⁻	-31.87		1	2 ^E	1	-31.47
5 ⁻	-29.31		5	3 ^E	1	-29.86
6 ⁻	-28.38		3	3 ^{A₁}	3	-28.11
7 ⁻	-25.87		3	4 ^{A₁}	3	-25.86
8 ⁻	-24.86		3	5 ^{A₁}	0	-24.57
0 ⁺	-35.04	A_1'	4	1 ^E	0	-35.47
1 ⁺	-34.19		2	1 ^E	1	-34.60
2 ⁺	-30.07		4	2 ^E	1	-30.45
3 ⁺	-27.03		2	3 ^E	0	-27.48
4 ⁺	-25.86		4	3 ^E	1	-25.91

corresponding energy levels for a $J \leq 5$ total angular momentum. The negligible differences in energy with those reported calculations show the capabilities of the present approach. In addition to this, the use of symmetry adapted vibrational basis set and the procedure to assign the corresponding symmetry character to the rovibrational $J > 0$ energy levels enables a complete description of the spectra of these kind of systems. The obtained results are as good as those previously reported for the Ar trimer. For Ne₃ the contribution from Coriolis distortion terms, found relevant in a previous investigation for the much lighter system H₃⁺, does not seem to be important.

5 Authors contributions

All the authors were involved in the preparation of the manuscript. All the authors have read and approved the final manuscript.

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