Collective rotations of asymmetrically deformed many-body systems. II. Intrinsic symmetry effects

1983 J. Phys. A: Math. Gen. 16 3197

(http://iopscience.iop.org/0305-4470/16/14/015)

J. Phys. A: Math. Gen. 16 (1983) 3197–3205. Printed in Great Britain

Collective rotations of asymmetrically deformed many-body systems: II. Intrinsic symmetry effects

Lucas F Lathouwers†

Dienst Teoretische en Wiskundige Natuurkunde, University of Antwerp (RUCA), Groenenborgerlaan 171, 2020 Antwerp, Belgium

Received 7 March 1983

Abstract. The implications of intrinsic symmetries on the structure of rotational secular equations in the angular momentum projection formalism are studied for both the exact and approximate versions. The symmetry group of the rigid rotor, D_2, is used to illustrate formal results.

1. Introduction

In paper I (Lathouwers and Deumens 1982) we developed an approximate angular momentum projection technique for asymmetrically deformed systems. The results obtained in I put angular momentum projection, as a means to insure rotational invariance, on a par with frame transformation theory (see e.g. Harter *et al* 1978). Indeed, although it is always possible to formally apply projection methods, approximate rotational energy level expressions in terms of quantum numbers, moments of inertia, centrifugal distortion constants, ... were available for axially symmetric systems only (Peierls and Yoccoz 1957, Verhaar 1964). The Peierls–Yoccoz approach was generalised in I by showing that for any strongly deformed intrinsic state the rotational secular equation reduces in a natural way to a rigid rotor eigenvalue problem. Since strong deformation is a property which occurs for both rigid and non-rigid systems, a qualitative explanation was obtained for the appearance of rotor-like energy level patterns in a large variety of many-body systems ('normal' or semi-rigid molecules, flexible molecules, Van der Waals complexes, atomic nuclei, ...). For a concise definition of the deformation of a wavefunction we refer to I. Here it suffices to say that if the overlap integral between a state and the one obtained from it by a non-infinitesimal rotation is vanishingly small it may be considered strongly deformed. It is easy to convince oneself that both for semi-rigid molecules, in which nuclei are strongly localised near the equilibrium configuration, and for heavy nuclei, in which nucleons are very delocalised as constituents of a determinental wavefunction, the above criterion is satisfied. Finally, it should be noted that I also introduced a quantal inertia tensor expressed in terms of the full microscopic Hamiltonian, total angular momentum components and the intrinsic wavefunction. The quantal inertia tensor

† Visiting Fellow at Harvard University during the 1982–1983 academic year. Present address: Department of Chemistry, Harvard University, Oxford Street 12, Cambridge, Massachusetts 02138, USA. Research Associate at the Nationaal Fonds voor Wetenschappelijk Onderzoek, Belgium.

turns out to be the proper concept for the quantitative description of collective rotational spectra since its eigenvalues are the moments of inertia appearing in the effective rigid rotor matrix equation. It, therefore, becomes possible to compute moments of inertia for systems that do not posess a preferred particle configuration.

Frequently intrinsic functions are derived from model Hamiltonians which have their proper symmetry groups e.g., molecular point groups, permutational symmetries, ... In this paper we will study the effect of such intrinsic symmetries on the projection operator treatment of overall rotation symmetry. It will be shown that if the invariance group of the intrinsic state contains rotations, linear dependencies among the projected matrix elements arise. Furthermore, we will verify that approximate angular momentum projection, as described in I, conserves the effects of intrinsic symmetry, i.e., the same relationships exist between exact and approximate forms of the projected matrix elements. The point group D_2, of special interest in both molecular (Kroto 1975) and nuclear physics (Bohr and Mottelson 1975), will serve to illustrate both the exact proof and the approximate version of the intrinsic symmetry effects.

Although some of the results of this paper are well known it is hoped that their transparent derivation within the projection operator formalism will stimulate further use of this technique as applied to non-rigid systems for which it seems ideally suited.

2. Symmetry properties of exactly projected matrix elements

When the general theory of projection operators is applied to the three-dimensional rotation group one obtains the so-called angular momentum projection operators

$$P^J_{MK} = \frac{2J+1}{8\pi^2} \int d\Omega\, D^{J*}_{MK}(\Omega)\mathscr{R}(\Omega) \tag{1}$$

$$d\Omega \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\gamma, \qquad \mathscr{R}(\Omega) \equiv \exp(-i\varphi J_z)\exp(-i\theta J_y)\exp(-i\gamma J_z) \tag{2}$$

$$D^J_{MK}(\Omega) \equiv D^J_{MK}(\varphi, \theta, \gamma) = \exp(-iM\varphi) d^J_{MK}(\theta) \exp(-iK\gamma) \tag{3}$$

where $\mathscr{R}(\Omega)$ and $D^J_{MK}(\Omega)$ are the rotation operators and rotation matrices expressed in terms of Euler angles $\Omega \equiv (\varphi, \theta, \gamma)$. The numerical factor $(2J+1)/8\pi^2$ is the ratio of the dimension of the irreducible representation J and the group volume $8\pi^2 \equiv \int d\Omega$. Formula (1) displays the general form of projection operators associated with a certain group if one observes that P^J_{MK} is the sum over the group of the group elements with the corresponding elements of the irreducible representations as coefficients. The usefulness of the P^J_{MK} lies in the fact that when applied to an arbitrary state $\chi(x)$ they generate, for each K, an eigenfunction of J^2 and J_z with associated quantum numbers J and M. Therefore, the most general wavefunction consistent with rotational invariance that can be extracted from $\chi(x)$ is

$$\Psi_{JM}(x) = \sum_K c^J_K P^J_{MK}\chi(x) = \frac{2J+1}{8\pi^2} \sum_K c^J_K \int d\Omega\, D^{J*}_{MK}(\Omega)\mathscr{R}(\Omega)\chi(x). \tag{4}$$

The superposition coefficients of the various K components can be determined by minimising the energy of $\Psi_{JM}(x)$ which leads to the following matrix eigenvalue problem (see e.g. Ring and Schuck 1980, MacDonald 1970)

$$\sum_L [H^J_{KL} - E^J \Delta^J_{KL}] c^J_L = 0 \tag{5}$$

$$H^J_{KL} = \langle\chi|HP^J_{KL}|\chi\rangle = \frac{2J+1}{8\pi^2}\int d\Omega\, D^{J*}_{KL}(\Omega)\langle\chi|H\mathscr{R}(\Omega)|\chi\rangle \tag{6}$$

$$\Delta^J_{KL} = \langle\chi|P^J_{KL}|\chi\rangle = \frac{2J+1}{8\pi^2}\int d\Omega\, D^{J*}_{KL}(\Omega)\langle\chi|\mathscr{R}(\Omega)|\chi\rangle. \tag{7}$$

In the introduction we referred to (5) as the rotational secular equation since for each total angular momentum value J a manifold of $2J+1$ rotational energy levels is obtained.

Suppose now that there exists an intrinsic symmetry group of which some elements are pure rotations. Without loss of generality† we consider the case in which $\chi(x)$ is invariant under a rotation $\mathscr{R}(\Omega_0)$ in the sense that

$$\mathscr{R}(\Omega_0)\chi(x) = r_0\chi(x) \qquad \text{with } |r_0|^2 = 1. \tag{8}$$

In order to examine the implications of (8) we need some extra properties of angular momentum projection operators namely

$$P^J_{KL}\mathscr{R}(\Omega_0) = \sum_M P^J_{KM} D^J_{LM}(\Omega_0) \qquad P^J_{KL}\mathscr{R}^+(\Omega_0) = \sum_M P^J_{KM} D^{J+}_{LM}(\Omega_0). \tag{9}$$

Although unfamiliar to most standard texts (see however Harter *et al* 1978), these equations are easily proved using definition (1) and the properties of Wigner functions. They allow us immediately to write down the relationship between the projected matrix elements we are aiming for. Indeed, it follows from (8) and (9) that

$$H^J_{KL} = r_0^* \sum_M H^J_{KM} D^J_{LM}(\Omega_0) \qquad H^J_{KL} = r_0 \sum_M H^J_{KM} D^{J+}_{LM}(\Omega_0) \tag{10}$$

if the intrinsic state is invariant under $\mathscr{R}(\Omega_0)$. Clearly similar equations hold for the overlap matrix elements Δ^J_{KL} although here and in the following we will not denote them explicitly. Thus both for H and Δ a projected matrix element is a linear combination of the elements of the same row with coefficients determined by the corresponding rotation matrix $D^J(\Omega_0)$.

We illustrate the above formal exposé for the group D_2 which is believed to be a near exact intrinsic symmetry group for asymmetric top molecules and triaxial nuclei. It contains the identity and the rotations over π around the three space fixed axes $\mathscr{R}(\pi, \bar{e}_k)$. The invariance property (8) can be written as

$$\mathscr{R}(\pi, \bar{e}_k)\chi(x) = r_k\chi(x) \tag{11}$$

where $r_k = \pm 1$. We now take into account various ways in which the $\mathscr{R}(\pi, \bar{e}_k)$ can be written in the Euler form (2) as summarised in table 1. Substitution in (10) gives us the following results

$$H^J_{KL} = r_x(-)^J H^J_{K-L} = r_x(-)^J H^J_{-KL} = H^J_{-K-L} \tag{12}$$

$$H^J_{KL} = r_y(-)^{J+K} H^J_{K-L} = r_y(-)^{J+L} H^J_{-KL} = (-)^{K+L} H^J_{-K-L} \tag{13}$$

$$H^J_{KL} = r_z(-)^K H^J_{KL} = r_z(-)^L H^J_{KL} = (-)^{K+L} H^J_{KL}. \tag{14}$$

† If the intrinsic state is degenerate one should proceed as described in Laskowski and Löwdin (1972).

Table 1. Possible Euler angle combinations for D_2 group elements.

D_2 element	$(\varphi, \theta, \gamma)$ combination
$\mathscr{R}(\pi, \bar{e}_x)$	$(\pi, \pi, 0), (0, \pi, \pi)$
$\mathscr{R}(\pi, \bar{e}_y)$	$(0, \pi, 0), (\pi, \pi, \pi)$
$\mathscr{R}(\pi, \bar{e}_z)$	$(\pi, 0, 0), (0, 0, \pi)$

These equations contain a number of redundancies due to the fact that e.g. $\mathscr{R}(\pi, \bar{e}_y)\mathscr{R}(\pi, \bar{e}_z) = \mathscr{R}(\pi, \bar{e}_x), \ldots$. The relevant implications of the D_2 symmetry are the following. Clearly, according to (14), K and L must have the same parity which is determined by r_z: K and L must be even or odd depending on whether $r_z = +1$ or -1. Secondly (13) and the corresponding equalities for Δ^J_{KL} imply that the components of the eigenvectors of equation (5) must be such that

$$c^J_K = (-)^{J+K} r_y c^J_{-K}. \tag{15}$$

For a given intrinsic D_2 symmetry, i.e., a given set (r_x, r_y, r_z), one therefore obtains a reduced number of existing rigid rotor energy levels (see table 2). These results are familiar from the Bohr–Mottelson approach to nuclear collective motion. However, their derivation within this framework is rendered dubious by the use of a redundant set of variables; a long-standing criticism of the collective model. We have shown here that a concise and transparent derivation can be given using the properties of angular momentum projection operators.

Table 2. Number of existing rotational states for given total angular momentum J and D_2 intrinsic quantum numbers (r_x, r_y, r_z).

J	r_z	r_y	Number of states
Even	+	+	$\frac{1}{2}J + 1$
		−	$\frac{1}{2}J$
	−	+	$\frac{1}{2}J$
		−	$\frac{1}{2}J$
Odd	+	+	$\frac{1}{2}(J - 1)$
		−	$\frac{1}{2}(J + 1)$
	−	+	$\frac{1}{2}(J + 1)$
		−	$\frac{1}{2}(J + 1)$

3. Symmetry properties of approximately projected matrix elements

Here we investigate whether the symmetry properties derived in the previous paragraph remain valid or are modified by introducing approximations appropriate for strongly deformed intrinsic states. For this purpose we will adopt the following strategy. In I it was shown that infinitesimal rotations essentially determine the angular momentum projected matrix elements. Approximate expressions in terms of angular momentum quantum numbers and components of the quantal inertia tensor were obtained. Clearly, if the intrinsic state is invariant under a rotation $\mathscr{R}(\Omega_0)$, in the sense of (8), transformations near $\mathscr{R}(\Omega_0)$ will also contribute in the projection integrals, i.e.,

$$H^J_{KL} \cong H^J_{KL}[1] + \sum H^J_{KL}[\mathscr{R}(\Omega_0)] \tag{16}$$

where the sum runs over all intrinsic symmetry elements. The symbol $H^J_{KL}[\mathscr{R}(\Omega_0)]$ indicates the contribution to H^J_{KL} of the rotations infinitesimally close to $\mathscr{R}(\Omega_0)$.

Specialising to the D_2 group the above arguments imply that we must evaluate the contributions of rotations near the $\mathscr{R}(\pi, \bar{e}_k)$ into the integrals (6) and (7). Table 3 gives the location of the group elements in terms the Euler angle θ and the sum and difference angles $\varphi+\gamma$ and $\varphi-\gamma$. Thus the relevant rotations are contained in the upper and lower slice of a parallelepiped with base $0 \leq \varphi,\ \gamma \leq 2\pi$ and height $0 \leq \theta \leq \pi$ (see figure 1(a)). Within these slices the transformations near the D_2 elements are distributed as indicated in figures 1(b) and 1(c). The approximate evaluation of the projected matrix elements now amounts to the computation of

$$H^J_{KL} \cong H^J_{KL}[1] + \sum_k H^J_{KL}[\mathscr{R}(\pi, \bar{e}_k)] \tag{17}$$

where the various contributions are given by the integrals over the corresponding regions indicated in figure 1. It will suffice to establish the relationship between the $H^J_{KL}[\mathscr{R}(\pi, \bar{e}_k)]$ and $H^J_{KL}[1]$ since the latter have already been evaluated in I.

Let us first consider transformations near $\mathscr{R}(\pi, \bar{e}_z)$. From figure 2 one sees that if the original integration domain is cut at $\varphi = \pi$ and the left-hand side translated over 2π in the φ direction one obtains an arrangement which is topologically identical to the one for infinitesimal rotations. Due to periodicity this procedure does not affect the value of the integral. However, in order for the two regions to coincide, one has

Table 3. Location of D_2 group elements in the parallepiped $0 \leq \varphi,\ \gamma \leq 2\pi$ and $0 \leq \theta \leq \pi$

D_2 element	θ	$\varphi-\gamma$	$\varphi+\gamma$
1	0	—	$0, 2\pi, 4\pi$
$\mathscr{R}(\pi, \bar{e}_x)$	0	—	$\pi, 3\pi$
$\mathscr{R}(\pi, \bar{e}_y)$	π	$0, 2\pi, 4\pi$	—
$\mathscr{R}(\pi, \bar{e}_z)$	π	$\pi, 3\pi$	—

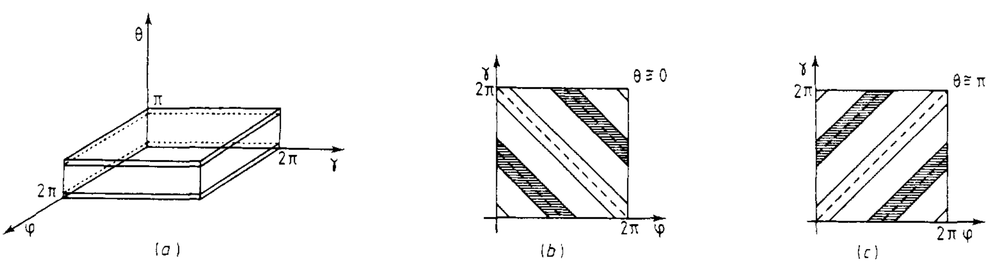

Figure 1. Location of D_2 group elements in the parallepiped $0 \leq \varphi,\ \gamma \leq 2\pi$ and $0 \leq \theta \leq \pi$. Near 1 and near $\mathscr{R}(\pi, \bar{e}_z)$ rotations in open and shaded regions of (b) respectively. Near $\mathscr{R}(\pi, \bar{e}_y)$ and near $\mathscr{R}(\pi, \bar{e}_x)$ rotations in open and shaded regions in (c) respectively.

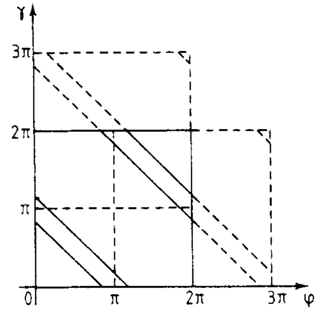

Figure 2. Integration domains relevant for the relationships between $H^J_{KL}[1]$ and $H^J_{KL}[\mathscr{R}(\pi, \bar{e}_z)]$.

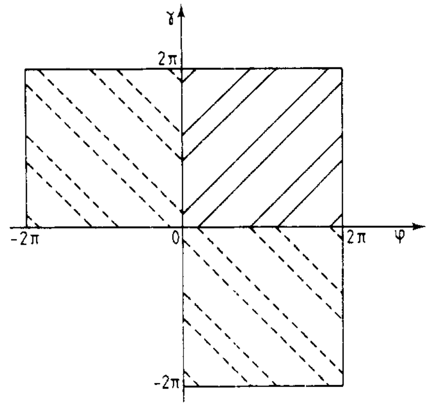

Figure 3. Integration domains relevant for the relationships between $H^J_{KL}[1]$ and $H^J_{KL}[\mathscr{R}(\pi, \bar{e}_y)]$, $H^J_{KL}[\mathscr{R}(\pi, \bar{e}_x)]$.

to translate the square $\pi \leqslant \varphi \leqslant 3\pi$, $0 \leqslant \gamma \leqslant 2\pi$ over $-\pi$ in the φ direction. This affects the integral by a phase factor which may be derived by considering the φ integration in the angular momentum projection. Indeed, the mathematics behind the above collage reads

$$\begin{aligned}
&\int_0^{2\pi} \mathrm{d}\varphi \, \exp(\mathrm{i}K\varphi) \ldots \langle \chi | \exp(-\mathrm{i}\varphi J_z) \ldots | \chi \rangle \\
&\qquad = \int_\pi^{3\pi} \mathrm{d}\varphi \, \exp(\mathrm{i}K\varphi) \ldots \langle \chi | \exp(-\mathrm{i}\varphi J_z) \ldots | \chi \rangle \\
&\qquad = \int_0^{2\pi} \mathrm{d}\varphi' \exp(-\mathrm{i}\pi K) \exp(\mathrm{i}K\varphi') \ldots \langle \chi | \exp(\mathrm{i}\pi J_z) \exp(-\mathrm{i}\varphi' J_z) \ldots | \chi \rangle \\
&\qquad = r_z(-)^K \int_0^{2\pi} \mathrm{d}\varphi' \exp(\mathrm{i}K\varphi') \ldots \langle \chi | \exp(-\mathrm{i}\varphi' J_z) \ldots | \chi \rangle .
\end{aligned} \tag{18}$$

Evidently the same procedure may be applied to the γ direction such that we conclude

$$H^J_{KL}[\mathscr{R}(\pi, \bar{e}_z)] = r_z(-)^K H^J_{KL}[1] = r_z(-)^L H^J_{KL}[1] = (-)^{K+L} H^J_{KL}[1]. \tag{19}$$

For rotations near $\mathscr{R}(\pi, \bar{e}_y)$ and $\mathscr{R}(\pi, \bar{e}_x)$ we observe that reflection with respect to the $\varphi(\gamma)$ axis followed by a translation over 2π in the $\gamma(\varphi)$ direction yields the same situation in the (φ, γ) plane as the one for infinitesimal and near $\mathscr{R}(\pi, \bar{e}_z)$ rotations. Figure 3 illustrates these operations. However, we still need an additional change of variables $\bar{\theta} = \pi - \theta$ to bring the upper slice of the parallelepiped into coincidence with the lower one. This results in a change in sign of one of the azimuthal quantum numbers and a phase factor. The explicit sequence of manipulations of the integrals is given in the appendix and proves that

$$H^J_{KL}[\mathscr{R}(\pi, \bar{e}_y)] = r_y(-)^{J+K} H^J_{K-L}[1] = r_y(-)^{J+L} H^J_{-KL}[1] = (-)^{K+L} H^J_{-K-L}[1] \tag{20}$$

$$H^J_{KL}[\mathscr{R}(\pi, \bar{e}_x)] = r_x(-)^J H^J_{K-L}[1] = r_x(-)^J H^J_{-KL}[1] = H^J_{-K-L}[1]. \tag{21}$$

We are now in a position to evaluate the approximate form of the full matrix element

H^J_{KL} by summing the four contributions from the D_2 group elements. Taking into account the relationships (19), (20) and (21) we obtain

$$H^J_{KL} \cong [1+r_z(-)^K](H^J_{KL}[1]+r_y(-)^{J+K}H^J_{-KL}[1]) \tag{22}$$

$$H^J_{KL} \cong [1+r_z(-)^L](H^J_{KL}[1]+r_y(-)^{J+L}H^J_{K-L}[1]). \tag{23}$$

These approximate forms do indeed satisfy the exact symmetry relations (12), (13) and (14). We may, therefore, conclude that approximate angular momentum projection conserves intrinsic symmetry effects.

The graphical methods, used in this section, clearly show that the D_2 symmetry effects arise from the interference between physically equivalent orientations of the intrinsic state. Indeed, summing over rotations near the D_2 group elements yields results equivalent to those obtained from the general projection operator properties (9).

4. Discussion

We have demonstrated that for D_2 intrinsic symmetries, the exact and approximate versions of angular momentum projection yield the same symmetry properties for the projected matrix elements. Their implications can be summarised by writing down the final wavefunctions taking account of (15), i.e.,

$$\Psi_{JMr}(x) = \sum_{K \geqslant 0} \frac{c^J_K}{1+\delta_{K0}}[P^J_{MK} + r_y(-)^{J+K}P^J_{M-K}]\chi_r(x) \tag{24}$$

where the sum runs over even or odd K values only and consistent with $r_z = (-)^K$. This equation gives us the number of states denoted in table 2 corresponding to a given total angular momentum J and intrinsic quantum numbers $r \equiv (r_x, r_y, r_z)$. That number and the form (24) are independent of whether the coefficient c^J_K are the solutions to the exact rotational secular equation (5) or the one corresponding to the approximate forms (22) and (23).

Looking at equation (13) from a group-theoretical point of view it is important to observe that the final wavefunctions are linear combinations of angular momentum eigenstates $P^J_{MK}\chi_r(x)$ which belong to the same irreducible representation of D_2 as the intrinsic states $\chi_r(x)$. We have emphasised this by assigning to both $\Psi_{JM}(x)$ and $\chi(x)$ the label $r \equiv (r_x, r_y, r_z)$. This statement is, in the present case, almost trivial because the intrinsic symmetry group D_2 is a subgroup of the overall symmetry group R_3 and has, in addition, only one-dimensional irreducible representations. The importance of the above observation lies in the fact that it hints to us which group-theoretical concepts are involved in treating the general situation in which a subgroup of both the intrinsic symmetry group and the overall symmetry group† is to be considered. Indeed, what we have gone through in this paper is nothing but an application of the theory of induced representations (Mackey 1968) which provides the general framework for problems of the type treated here. The present approach using projection operators and an explicit rotation group parametrisation in terms of Euler angles is however to be preferred at an introductory and practical level.

† In the absence of external fields one may want to include (in addition to rotations) translations, parity and time invariance, permutations of identical particles, ...

In addition to the question considered in the previous paragraphs, i.e., which wavefunctions are consistent with a given intrinsic symmetry, one should also ask oneself how the intrinsic symmetry affects the position of the corresponding energy levels. From (22) and (23) it is clear that the spectrum can no longer be that of the rigid rotor shown in I to be equivalent to the secular equations for $H^J_{KL}[1]$ and $\Delta^J_{KL}[1]$. Indeed, the latter matrix elements are modified by contributions of the form $r_y(-)^{J+{}^{L}_{K}} H^K_{\pm K,\mp L}[1]$ and $(-)^{J+{}^{L}_{K}}\Delta^J_{\pm K,\mp L}$. Due to the presence of the sign factor $(-)^J$ the resulting energy shifts will be different for even or odd J values. For axially symmetric systems these so-called odd–even shifts have been treated by Verhaar (1963). However, it can be seen that these effects are mixed with centrifugal distortion corrections which appear as higher-order expansions beyond the Gaussian overlap and quadratic approximations considered in I. Since this is the topic of the next paper in this series we will consider generalised odd–even shifts and centrifugal distortions simultaneously in a future publication.

Acknowledgments

This work was partly sponsored by the National Science Foundation (USA) through research grants at the University of Florida, Gainesville, Florida and Harvard University, Cambridge, Massachusetts. The author would like to thank Professors E B Wilson, W Klemperer, N Y Ohrn and P Van Leuven for continued interest in this project.

Corrigendum to Paper I

Lathouwers L F and Deumens E 1982 *J. Phys. A: Math. Gen.* **15** 2785–99

On page 2785, line four of the Introduction, 'quantitative' should read 'qualitative'.

In equation (19) on page 2789, the term on the RHS of the first equation should end as $e^{+i\delta J_z}\, e^{-i\varepsilon J_z}$.

In figure 1 a broken line from $(0, 2\pi)$ to $(2\pi, 0)$ is missing.

In equation (40) x and y should be interchanged.

On page 2799 in line eight $P^2_0(t)$ should be replaced by $P^0_2(t)$.

Appendix

We derive here the first equation (20) as an illustration of the mathematical manipulations behind the graphical approach used in § 3. In order to shorten the expressions we only denote the θ and γ integrations. One can then easily verify that

$$\int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\gamma\, d^J_{KL}(\theta) \exp(-iL\gamma)\langle\chi| \dots \exp(-i\theta J_y)\exp(-i\gamma J_z)|\chi\rangle$$

$$= \int_0^{\pi} \sin\theta'\, d\theta' \int_0^{2\pi} d\gamma\, d^J_{KL}(\pi-\theta')\exp(-iL\gamma)$$

$$\times \langle \chi | \ldots \exp(\mathrm{i}\theta' J_y) \exp(-\mathrm{i}\pi J_y) \exp(-\mathrm{i}\gamma J_z) | \chi \rangle$$

$$= (-)^{J+K} \int_0^{\pi} \sin\theta' \, \mathrm{d}\theta' \int_0^{2\pi} d\gamma \, d^J_{K-L}(\theta') \exp(-\mathrm{i}L\gamma)$$

$$\times \langle \chi | \ldots \exp(\mathrm{i}\theta' J_y) \exp(\mathrm{i}\gamma J_z) \exp(-\mathrm{i}\pi J_y) | \chi \rangle$$

$$= r_y (-)^{J+K} \int_0^{\pi} \sin\theta' \, \mathrm{d}\theta' \int_0^{2\pi} \mathrm{d}\gamma' \, d^J_{K-L}(\theta') \exp(\mathrm{i}L\gamma')$$

$$\times \langle \chi | \ldots \exp(\mathrm{i}\theta' J_y) \exp(-\mathrm{i}\gamma' J_z) | \chi \rangle$$

$$= r_y (-)^{J+K} \int_0^{\pi} \sin\theta' \, \mathrm{d}\theta' \int_0^{2\pi} \mathrm{d}\gamma' \, d^J_{K-L}(\theta')$$

$$\times \exp(\mathrm{i}L\gamma') \langle \chi | \ldots \exp(-\mathrm{i}\theta' J_y) \exp(-\mathrm{i}\gamma' J_z) | \chi \rangle$$

where the last line follows from

$$\langle \chi | \exp(-\mathrm{i}\varphi J_z) \exp(\mathrm{i}\theta' J_y) \exp(-\mathrm{i}\gamma' J_z) | \chi \rangle$$

$$= \langle \chi | \exp(\mathrm{i}\pi J_z) \exp(-\mathrm{i}\varphi J_z) \exp(-\mathrm{i}\pi J_z) \exp(\mathrm{i}\theta' J_y)$$

$$\times \exp(\mathrm{i}\pi J_z) \exp(-\mathrm{i}\gamma' J_z) \exp(-\mathrm{i}\pi J_z) | \chi \rangle$$

$$= r_z^2 \langle \chi | \exp(-\mathrm{i}\varphi J_z) \exp(-\mathrm{i}\theta' J_y) \exp(-\mathrm{i}\gamma' J_z) | \chi \rangle$$

$$= \langle \chi | \exp(-\mathrm{i}\varphi J_z) \exp(-\mathrm{i}\theta' J_y) \exp(-\mathrm{i}\gamma' J_z) | \chi \rangle .$$

References

Bohr A and Mottelson B 1975 *Nuclear Structure* vol II (Reading, Mass: Benjamin)
Harter W G *et al* 1978 *Rev. Mod. Phys.* **50** 37
Kroto H W 1975 *Molecular Rotation Spectra* (New York: Wiley)
Laskowski B and Löwdin P O 1972 *Chem. Phys. Lett.* **16** 1
Lathouwers L and Deumens E 1982 *J. Phys. A: Math. Gen.* **15** 2785
MacDonald N 1970 *Adv. Phys.* **19** 371
Mackey G W 1968 *Induced Representations of Groups and Quantum Mechanics* (New York: Benjamin)
Peierls R E and Yoccoz J 1957 *Proc. Phys. Soc.* **A70** 381
Ring P and Schuck P 1980 *The Nuclear Many-Body Problem* (New York: Springer)
Vehaar B 1963 *Nucl. Phys.* **45** 129
—— 1964 *Nucl. Phys.* **54** 641