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Lie algebra projectors and the kinematics of collective motions

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Abstract. Direct-sum decompositions of the Euclidean space of particle momenta into collective and intrinsic subspaces are achieved using projectors on so(3) and gl(3, R) algebra spaces. The separation of the N-particle kinetic energy into the corresponding collective and intrinsic components is then simply obtained. In the case of gl(3, R) the resulting intrinsic kinetic energy is expressed in terms of an appropriate subset of the generators of the direct product group $\mathrm{SO}(N)\times\mathrm{SO}(N)$. A detailed comparison of these results with those of other authors is given.

1. Introduction

The Bohr–Mottelson nuclear collective model (Bohr 1952, Bohr and Mottelson 1953, Bohr *et al* 1976) has been widely and successfully used to describe nuclear collective properties. To put this model on a microscopic foundation a number of authors have performed a transformation from the particle coordinates to a set of collective and intrinsic coordinates. The end product of such a transformation may be viewed as expressing the particle momenta in terms of a set of collective and intrinsic momenta taken to be the generators of some Lie groups $\mathrm{G}_{\mathrm{coll}}$ and $\mathrm{G}_{\mathrm{intr}}$ respectively†. To describe rotational motion Villars (Villars 1957, Villars and Cooper 1970), Gupta and Skinner (1968), Rowe (1970) and Herold (Herold and Ruder 1979, Herold 1979) chose $\mathrm{G}_{\mathrm{coll}}=\mathrm{SO}(3)$. To include vibrational motion as well and obtain a microscopic analogue of the full Bohr–Mottelson collective model, Zickendraht (1971), Dzyublik *et al* (1972), Filippov (1974), Petrauskas and Sabalyauskas (1975), Ovcharenko (1976), Gulshani and Rowe (1976), Weaver *et al* (1976), Vanagas (1977), Gulshani (1978) and Buck *et al* (1979) chose $\mathrm{G}_{\mathrm{coll}}=\mathrm{GL}(3,\mathrm{R})$, the general linear group in three real dimensions.

Having chosen $\mathrm{G}_{\mathrm{coll}}=\mathrm{GL}(3,\mathrm{R})$, one now faces the problem of finding an appropriate set of intrinsic momenta consistent with the collective and the original momenta. Dzyublik *et al* (1972) and Ovcharenko (1976) have derived expressions for the intrinsic momenta and the intrinsic kinetic energy of the N-particle system in terms of a subset of the generators of the orthogonal group $\mathrm{SO}(N-1)$ in some abstract N-dimensional space. In this paper we give a geometrically simple and clear derivation of the separation of the particle momenta and the total kinetic energy into collective and intrinsic components using projection operators on Lie algebra spaces.

† We follow, in this paper, the common designation of reserving capital letters for the group and lower case letters for the corresponding Lie algebra.

In § 3 the projection operator on the so(3) vector space is defined and the corresponding collective rotational kinetic energy is derived in § 4. In § 5 we study the group that is of interest to us in this paper, namely GL(3, R). The projection operator on the Lie algebra gl(3, R) is defined and used in § 6 to project out the corresponding collective kinetic energy of an N-particle system. In § 7 the corresponding intrinsic kinetic energy component is then expressed in terms of a set of $3N$ intrinsic momenta which are generators of the group SO(N). A discussion of why these intrinsic momenta are not all independent and hence not appropriate is given. Finally, in § 8 we use Ovcharenko's (1976) approach to find an appropriate set of $3N-9$ intrinsic momenta as a subset of the generators of the direct product group SO(N)$\times$SO(N) of an N-dimensional asymmetric top, in some abstract N-dimensional space. Comparison with the works of other authors is also given.

2. Coordinate transformations and projectors

Consider the $3N$-dimensional Euclidean space $\mathbb{R}^{3N}$ of the N-particle Cartesian coordinates x_{ni} $(n=1,\ldots,N; i=1,2,3)$ and the corresponding space $\mathbb{P}^{3N}$ of the quantum-mechanical momenta $p_{ni}\equiv -i\hbar\partial/\partial x_{ni}$. The total kinetic energy of the N-particle system is

$$T\equiv\frac{1}{2M}\sum_{n=1}^{N}\sum_{i=1}^{3}p_{ni}^2$$

where M is the mass of each particle. Consider next a transformation on $\mathbb{R}^{3N}$ which decomposes $\mathbb{P}^{3N}$ into a sum of collective $\mathbb{P}_{\text{coll}}$ and intrinsic $\mathbb{P}_{\text{intr}}$ subspaces and write, for $p_{ni}\in\mathbb{P}^{3N}$, $p_{ni}=p_{ni}^{\text{intr}}+p_{ni}^{\text{coll}}$ where $p_{ni}^{\text{intr}}\in\mathbb{P}_{\text{intr}}$ and $p_{ni}^{\text{coll}}\in\mathbb{P}_{\text{coll}}$. the transformation may be chosen so that p_{ni}^{coll} is a linear combination of the generators of some relevant Lie group G_{coll}. Then $\mathbb{P}_{\text{coll}}$ coincides with the Lie algebra space of G_{coll}.

A most desirable situation arises when the above decomposition is a direct sum, i.e. $\mathbb{P}^{3N}=\mathbb{P}_{\text{intr}}\oplus\mathbb{P}_{\text{coll}}$ with $\mathbb{P}_{\text{intr}}$ and $\mathbb{P}_{\text{coll}}$ having no vectors in common and being mutually orthogonal. This is a generalisation of the concept of orthogonality of p_{ni}^{intr} and p_{ni}^{coll} and would result, in classical mechanics, in the vanishing of the terms $\Sigma_{ni}p_{ni}^{\text{intr}}p_{ni}^{\text{coll}}$ in the transformed kinetic energy T. Such a decomposition is achieved very simply using the projection techniques (Pease 1965, Finkbeiner 1960). Specificially, one looks for a projection operator Γ which carries every element p_{ni} of $\mathbb{P}^{3N}$ into an element of the Lie algebra space of G_{coll}. One then obtains a simply and explicitly $p_{ni}^{\text{coll}}=\Gamma p_{ni}$ and $p_{ni}^{\text{intr}}=(1-\Gamma)p_{ni}$.

In the derivations that follow below we ignore throughout the motion of the centre of mass. This, however, can be accounted for by minor changes in the definitions of the quantities that occur.

3. Projector for $G_{\text{coll}}=SO(3)$

The three generators L_i $(i=1,2,3)$ of SO(3) span a three-dimensional vector space so(3) over a field F. In $\mathbb{R}^{3N}L_i$ can be realised by the angular momentum differential operators

$$L_k=\sum_{n=l}^{N}\epsilon_{kij}x_{ni}p_{nj} \tag{3.1}$$

where ϵ_{kij} is the unit antisymmetric third-rank tensor. Now we define in $\mathbb{R}^{3N}$ the Hermitian operator (summation over repeated indices is implied throughout)

$$\Gamma^{(3)}_{ni,mj} \equiv -MZ^{(k)}_{ni}\mathcal{I}^{-1}_{kl}Z^{(l)}_{mj} \tag{3.2}$$

where

$$Z^{(k)}_{ni} \equiv \epsilon_{kij}x_{nj} \tag{3.3}$$

and $\mathcal{I}^{-1}$ is the inverse of the rigid-body tensor defined by

$$\mathcal{I}_{ij} \equiv (\mathrm{Tr}\ Q)\delta_{ij} - Q_{ij} \tag{3.4}$$

and Q_{ij} is the mass quadrupole tensor defined by

$$Q_{ij} \equiv Mx_{ni}x_{nj}. \tag{3.5}$$

We claim that $\Gamma^{(3)}$ in (3.2) is a projector on so(3), i.e. carries every element p_{ni} of $\mathbb{P}^{3N}$ into an element of so(3). The proof is as follows.

First observe that the space spanned by the three $3N$-dimensional vectors $Z^{(k)}_{ni}$ in (3.3) is invariant under $\Gamma^{(3)}$, i.e.

$$\Gamma^{(3)}_{ni,mj}Z^{(k)}_{mj} = Z^{(k)}_{ni}. \tag{3.6}$$

Equation (3.6) is easily proved using equations (3.4), (3.5) and the identity $\epsilon_{\tilde{k}ij}\epsilon_{\tilde{k}lk} \equiv \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl}$. Now it is easy to show that

$$\mathrm{Tr}\,\Gamma^{(3)} \equiv \sum_{n=1}^{N}\sum_{i=1}^{3}\Gamma_{ni,ni} = 3 \tag{3.7}$$

$$\Gamma^{(3)2}_{ni,mj} = \Gamma^{(3)}_{ni,\tilde{m}\tilde{k}}\Gamma^{(3)}_{\tilde{m}\tilde{k},mj} = \Gamma^{(3)}_{ni,mj}, \tag{3.8}$$

i.e. $\Gamma^{(3)}$ has rank three and is idempotent. We define the projection in $\mathbb{P}^{3N}$ by

$$p^{\mathrm{rot}}_{ni} \equiv \Gamma^{(3)}_{ni,mj}p_{mj} \tag{3.9}$$

and

$$p^{\mathrm{rot}} \equiv \Gamma^{(3)}(p).$$

Then for an arbitrary vector $l_{a_k} \equiv a_kL_k = a_k\epsilon_{kij}x_{ni}p_{nj} \in \mathrm{so}(3)$ with $a_k \in F$ we have, from equations (3.9) and (3.6),

$$\begin{aligned}(l_{a_k})^{\mathrm{rot}} &\equiv \Gamma^{(3)}(l_{a_k}) \equiv a_k\epsilon_{kij}x_{ni}p^{(\mathrm{rot})}_{nj}\\ &= a_k\epsilon_{kij}x_{ni}\Gamma^{(3)}_{nj,ml}p_{ml}\\ &= a_k\epsilon_{kjl}x_{mj}p_{ml} = l_{a_k}.\end{aligned} \tag{3.10}$$

Equation (3.10) shows that so(3) is invariant under $\Gamma^{(3)}$. For a vector u orthogonal to l_{a_k}, i.e. $u\,.\,l_{a_k} = 0$, its projection is also orthogonal to l_{a_k}, i.e.

$$\begin{aligned}\Gamma^{(3)}(u)\,.\,l_{a_k} &= u\,.\,\Gamma^{(3)}(l_{a_k})\\ &= u\,.\,l_{a_k} \equiv 0.\end{aligned} \tag{3.11}$$

From equations (3.7), (3.8), (3.10) and (3.11) it follows (Pease 1965, Finkbeiner 1960) that $\Gamma^{(3)}$ is indeed a projector of $\mathbb{P}^{3N}$ on so(3).

4. Kinetic energy for rotation

Since the operator $\Gamma^{(3)}$ in equation (3.2) projects every element p_{ni} of the Cartesian momentum space $\mathbb{P}^{3N}$ on the Lie algebra space of SO(3), we readily obtain the decomposition

$$p_{ni} \equiv p_{ni}^{\text{intr}} + p_{ni}^{\text{rot}}$$
$$\equiv (\delta_{mn}\delta_{ij} - \Gamma^{(3)}_{ni,mj})p_{mj} + \Gamma^{(3)}_{ni,mj}p_{mj} \tag{4.1}$$

for the rotational motion. The importance of the apparently trivial identity in (4.1) lies in the expression for p_{ni}^{rot}, which can easily be expressed as

$$p_{ni}^{\text{rot}} \equiv \Gamma^{(3)}_{ni,mj}p_{mj} \equiv -M(\boldsymbol{x}_n \times (\mathscr{I}^{-1}.\boldsymbol{L}))_i \tag{4.2}$$

where the definition of $\Gamma^{(3)}$ in equation (3.2) has been used and $\boldsymbol{L}$ is the angular momentum vector. Equation (4.2) is merely the 'rigid'-body rotation expression for the collective components of the individual particle momenta.

In classical mechanics p_{ni}^{intr} and p_{ni}^{rot} in equation (4.1) are, by construction, orthogonal in the sense that $\Sigma_{ni}p_{ni}^{\text{intr}}p_{ni}^{\text{coll}} = 0$. This is not so in quantum mechanics because p_{ni} are differential operators on $\mathbb{R}^{3N}$ and hence do not commute with $\Gamma^{(3)}$. Nevertheless, in the corresponding decomposition of the kinetic energy T, obtained from equation (4.1), these cross terms can readily be seen to vanish trivially. One therefore obtains the clean decomposition

$$T \equiv \frac{1}{2M}\sum_{ni} p_{ni}^2 \equiv T_{\text{intr}} + T_{\text{rot}}$$
$$= \frac{1}{2M} p_{ni}(\delta_{nm}\delta_{ij} - \Gamma^{(3)}_{ni,mj})p_{mj} + \frac{1}{2M} p_{ni}\Gamma^{(3)}_{ni,mj}p_{mj}. \tag{4.3}$$

Now it is simple to show that

$$T_{\text{rot}} \equiv \frac{1}{2M} p_{ni}\Gamma^{(3)}_{ni,mj}p_{mj} = \tfrac{1}{2}\boldsymbol{L}.\mathscr{I}^{-1}.\boldsymbol{L}, \tag{4.4}$$

which is the 'rigid'-body rotation kinetic energy. The properties of $\Gamma^{(3)}$, p_{ni}^{intr} and T_{intr} in equations (3.2), (4.1) and (4.3) will be examined in detail in a forthcoming publication. Our main concern here is, however, the kinematic group GL(3, R) to which we now turn.

5. Projector for $G_{\text{coll}} = \text{GL}(3, \text{R})$

The nine generators $t_{ij}(i, j = 1, 2, 3)$ of the group GL(3, R) span a nine-dimensional vector space gl(3, R) over a field F. An arbitrary element of gl(3, R) acting on $\mathbb{R}^{3N}$ is realised by

$$t_{a_{ij}} \equiv \sum_{i,j=1}^{3} a_{ij}t_{ij} \equiv \sum_{i,j=1}^{3} a_{ij} \sum_{n=1}^{N} x_{ni}p_{nj} \tag{5.1}$$

with $a_{ij} \in F$. Let us define the Hermitian operator

$$\Gamma^{(9)}_{ni,mj} \equiv M\delta_{ij}x_{nk}Q^{-1}_{kl}x_{ml} \tag{5.2}$$

where Q^{-1} is the inverse of the quadrupole tensor (3.5) and the summation over repeated indices in (5.2) and throughout is implied. We claim that $\Gamma^{(9)}_{ni,mj}$ in (5.2) is a projector on gl(3, R) of the elements p_{ni} of $\mathbb{P}^{3N}$. The proof is as follows.

From equations (5.2) and (3.5) we have

$$\operatorname{Tr}\Gamma^{(9)} \equiv \sum_{ni} \Gamma^{(9)}_{ni,ni} = 9 \tag{5.3}$$

$$\Gamma^{(9)2}_{ni,mj} \equiv \Gamma^{(9)}_{ni,\tilde{m}\tilde{l}}\Gamma^{(9)}_{\tilde{m}\tilde{l},mj} = \Gamma^{(9)}_{ni,mj} \tag{5.4}$$

i.e. $\Gamma^{(9)}$ has rank nine and is idempotent, and

$$\Gamma^{(9)}_{ni,mj}x_{ml} = \delta_{ij}x_{nl}. \tag{5.5}$$

Let us define the projection in $\mathbb{P}^{3N}$ by

$$p^{\text{coll}}_{ni} = \Gamma^{(9)}_{ni,mj}p_{mj} \tag{5.6}$$

or

$$p^{\text{coll}} = \Gamma^{(9)}(p).$$

Then for the arbitrary vector (5.1) of gl(3, R) we have

$$\begin{aligned} t^{\text{coll}}_{a_{ij}} &\equiv \Gamma^{(9)}(t^{\text{coll}}_{a_{ij}}) = a_{ij}x_{ni}p^{\text{coll}}_{nj} \\ &\equiv t_{a_{ij}} \end{aligned} \tag{5.7}$$

where equations (5.5) and (5.6) have been used. For any vector u orthogonal to $t_{a_{ij}}$, i.e. $u\,.\,t_{a_{ij}} = 0$, its projection $\Gamma^{(9)}u$ is also orthogonal to $t_{a_{ij}}$, i.e.

$$\begin{aligned} \Gamma^{(9)}(u)\,.\,t_{a_{ij}} &= u\,.\,\Gamma^{(9)}(t_{a_{ij}}) \\ &= u\,.\,t_{a_{ij}} \equiv 0. \end{aligned} \tag{5.8}$$

Equations (5.3), (5.4), (5.7) and (5.8) show that $\Gamma^{(9)}_{ni,mj}$ in (5.2) is, indeed, a projector on the vector space gl(3, R).

The Kronecker delta δ_{ij} in (5.2) plays no role in what follows and we choose to omit it and redefine the gl(3, R) projector (5.2) as

$$\Gamma_{nm} \equiv Mx_{ni}Q^{-1}_{ij}x_{mj}. \tag{5.9}$$

Equation (5.5) then reduces to

$$\Gamma_{nm}x_{mi} = x_{ni}. \tag{5.10}$$

6. Kinetic energy for rotation and vibration

Since Γ_{nm} in (5.9) projects the Cartesian momentum space $\mathbb{P}^{3N}$ on the space spanned by the Lie algebra of GL(3, R), one readily obtains, for the rotation–vibrational motion described by GL(3, R), the decomposition

$$\begin{aligned} p_{ni} &\equiv p^{\text{intr}}_{ni} + p^{\text{coll}}_{ni} \\ &\equiv (\delta_{mn} - \Gamma_{nm})p_{mi} + \Gamma_{nm}p_{mi}. \end{aligned} \tag{6.1}$$

In classical mechanics p^{intr}_{ni} and p^{coll}_{ni} are, by construction, orthogonal in the sense that $\Sigma_{ni}p^{\text{intr}}_{ni}p^{\text{coll}}_{ni} = 0$. This is not the case in quantum mechanics as p_{ni} and Γ_{nm} do not commute. Nevertheless, in the total kinetic energy T these cross terms vanish as a simple consequence of the definition (6.1) and one readily obtains the clean decomposition

$$T \equiv \frac{1}{2M} \sum_{i=1}^{N} \sum_{i=1}^{3} p_{ni}^2$$
$$\equiv T_{\text{intr}} + T_{\text{coll}} \tag{6.2a}$$

where

$$T_{\text{intr}} \equiv \frac{1}{2M} p_{ni}(\delta_{nm} - \Gamma_{nm}) p_{mi} \tag{6.2b}$$

and

$$T_{\text{coll}} \equiv \frac{1}{2M} p_{ni} \Gamma_{nm} p_{mi}. \tag{6.2c}$$

Clearly p_{ni}^{coll} and T_{coll} in (6.1) and (6.2c) are projected components in GL(3, R) Lie algebra space since, from equation (5.9), one can write

$$p_{ni}^{\text{coll}} \equiv \Gamma_{nm} p_{mi} = M x_{nj} Q_{jk}^{-1} t_{ki} \tag{6.3}$$

and

$$T_{\text{coll}} \equiv \frac{1}{2M} p_{ni} \Gamma_{nm} p_{mi} = \tfrac{1}{2} \operatorname{Tr} (\tilde{t} \,.\, Q^{-1} \,.\, t - \mathrm{i}\hbar N Q^{-1} \,.\, t) \tag{6.4}$$

where t_{ij} are the nine generators of GL(3, R) defined in equation (5.1) and $\tilde{t}_{ij} \equiv t_{ji}$. Except for the effect of the omission of the centre-of-mass motion, expressions (6.3) and (6.4) are identical to those derived previously by the author (Gulshani and Rowe 1976, Gulshani 1977, 1978; see also Vanagas 1977) using coordinate transformation. In these works expression (6.4) has been studied in detail in connection with the spectrum generating algebras $\mathbb{R}^6 \otimes \mathrm{so}(3) \equiv \{Q_{ij}, L_k\}$, gl(3, R), $\mathrm{cm}(3) \equiv \{Q_{ij}, t_{ij}\}$ and the Heisenberg algebra $\{Q_{ij}, P_{lk}, I;\ [Q_{ij}, P_{lk}] = \mathrm{i}\hbar \delta_{il} \delta_{jk}\}$. In particular, we see that T_{coll} in (6.4) is a rational function of the algebra cm(3). This becomes obvious when the identity

$$Q_{ij}^{-1} = \frac{1}{2 \det Q} [(\operatorname{Tr} Q)^2 - \operatorname{Tr} Q^2 - 2(\operatorname{Tr} Q) Q + Q^2]_{ij},$$

where $\det Q$ is the determinant of Q, is used.

The physical meaning of T_{coll} becomes more apparent by transforming it to the quadrupole principal axis defined by the orthogonal transformation

$$R_{Ai} Q_{ij} R_{Bj} \equiv \delta_{AB} I_A \qquad (A, B = 1, 2, 3) \tag{6.5}$$

where $R \in \mathrm{SO}(3)$ and I_A are the three principal quadrupole moments defined by

$$I_A \equiv \sum_{n=1}^{N} x_{nA}^2. \tag{6.6}$$

In equation (6.6) x_{nA} are the principal-axis components of x_{ni} defined by

$$x_{nA} \equiv R_{Ai} x_{ni}. \tag{6.7}$$

T_{coll} in equation (6.4) can then be written as (Gulshani and Rowe 1976)

$$T_{\text{coll}} \equiv T_{\text{vib}} + T_{\text{rot}} \tag{6.8a}$$

where

$$T_{\text{vib}} \equiv -2\hbar^2 \sum_{A=1}^{3} I_A \left[\frac{\partial^2}{\partial I_A^2} + \left(\frac{N-2}{2I_A} + \sum_{B \neq A}^{3} \frac{1}{I_A - I_B}\right)\frac{\partial}{\partial I_A}\right] \tag{6.8b}$$

$$T_{\text{rot}} \equiv \tfrac{1}{2} \sum_{A<B}^{3} \left(\frac{I_A + I_B}{(I_A - I_B)^2}(L_{AB}^2 + \mathscr{L}_{AB}^2) - \frac{4(I_A I_B)^{1/2}}{(I_A - I_B)^2} L_{AB}\mathscr{L}_{AB}\right). \tag{6.8c}$$

The operators appearing in (6.8*b*, *c*) are defined in terms of the principal-axis components

$$t_{AB} \equiv R_{Ai} R_{Bj} t_{ij} \tag{6.9}$$

of t_{ij} in (5.1) as follows (Gulshani and Rowe 1976):

$$L_{AB} \equiv t_{AB} - t_{BA} \tag{6.10}$$

$$-\mathrm{i}\hbar\partial/\partial I_A \equiv \tfrac{1}{2} t_{AA} \tag{6.11}$$

$$\mathscr{L}_{AB} \equiv (I_B/I_A)^{1/2} t_{AB} - (I_A/I_B)^{1/2} t_{BA}. \tag{6.12}$$

Equations (6.10)–(6.12) define respectively the principal-axis components of the angular momentum, dilation momenta and 'vortex' angular momentum. In deriving (6.8 b, c) from equation (6.4) we have used the fact that $[L_{AB}, \mathscr{L}_{CD}] = [L_{AB}, I_C] = [\mathscr{L}_{AB}, I_C] = 0$. A detailed study of the expressions in equations (6.8*b*, *c*) is given by the author (Gulshani and Rowe 1976, Gulshani 1978).

7. The intrinsic kinetic energy

The decomposition of the particle momentum space $\mathbb{P}^{3N}$ into collective and intrinsic subspaces will be completed once we have found a set of $3N$–9 linearly independent intrinsic momenta in terms of which p_{ni}^{intr} can be expressed. A candidate for such a set appears to be a subset of the generators of the orthogonal group SO(N) (Morinigo 1972, Dzyublik *et al* 1972, Ovcharenko 1976). These generators may be realised on $\mathbb{R}^{3N}$ by the $\frac{1}{2}N(N-1)$ operators, the so called particle-index angular momentum (Morinigo 1972):

$$J_{nm} \equiv x_{ni} p_{mi} - x_{mi} p_{ni}. \tag{7.1}$$

Now using the identities

$$p_{mi} \equiv M Q_{ik}^{-1} x_{nk} x_{nl} p_{ml}$$

and

$$(\delta_{nm} - \Gamma_{nm}) x_{mi} \equiv 0$$

which follow respectively from equations (3.5) and (5.10), we obtain for the intrinsic components of the particle momenta, defined in (6.1), the expression

$$p_{ni}^{\text{intr}} \equiv \sqrt{M} Q_{ik}^{-1/2} \bar{J}_{nk} \tag{7.2}$$

where the $3N$ quantities $\bar{J}_{nk}$ are defined by

$$\bar{J}_{nk} \equiv (\delta_{nm} - \Gamma_{nm}) \bar{R}_{\bar{n}k} J_{\bar{n}m} \tag{7.3}$$

and

$$\bar{R}_{ni} \equiv \sqrt{M} x_{nk} Q_{ki}^{-1/2}. \tag{7.4}$$

We now use the commutation relation

$$[J_{nm}, x_{\tilde{n}i}] = -\mathrm{i}\hbar(\delta_{m\tilde{n}}x_{ni} - \delta_{n\tilde{n}}x_{mi}) \tag{7.5}$$

and, hence,

$$[J_{nm}, Q_{ij}] = [J_{nm}, R_{Ai}] = [J_{nm}, I_A] = 0 \tag{7.6}$$

to write

$$\begin{aligned} T_{\text{intr}} &\equiv \frac{1}{2M}\sum_{n=1}^{N}\sum_{i=1}^{3}(p_{ni}^{\text{intr}})^2 \\ &= \tfrac{1}{2}\bar{J}_{ni}Q_{ij}^{-1}\bar{J}_{nj}. \end{aligned} \tag{7.7}$$

Transforming (7.7) to the quadrupole principal axis given in equation (6.5) and using the relations

$$[J_{nm}, I_A] = [J_{nm}, R_{Ai}] = 0, \tag{7.8}$$

one readily obtains the expression

$$T_{\text{intr}} = \tfrac{1}{2}\sum_{n=1}^{N}\sum_{A=1}^{3}\frac{1}{I_A}\bar{J}_{nA}^2 \tag{7.9}$$

where

$$\bar{J}_{nA} \equiv R_{Ai}\bar{J}_{ni}. \tag{7.10}$$

By means of a simple manipulation one can also express the three generators $\mathscr{L}_{AB}$, in equations (6.12), of GL(3, R) in terms of the operators J_{nm} of SO(N) as follows:

$$\mathscr{L}_{AB} = \bar{R}_{nA}\bar{R}_{mB}J_{nm} \tag{7.11}$$

where

$$\bar{R}_{nA} = R_{Ai}\bar{R}_{ni} = (M/I_A)^{1/2}x_{nA}. \tag{7.12}$$

An expression for T_{intr} similar to that in equations (7.9) has been given by Rowe and Rosensteel (1979 a, b). But these two expressions are, in fact, quite different in detail. Whereas T_{intr} in (7.9) involves $3N$ intrinsic momenta $\bar{J}_{nA}$†, that given by Rowe and Rosensteel (1979a, b) involves $3N$–9 intrinsic momenta. Their set of $3N$–9 intrinsic momenta are defined differently from that of $\bar{J}_{nA}$ in equations (7.3) and (7.10). In fact, we show in appendix 2 that the set of $3N$–9 intrinsic momenta given by these authors does not have well defined action in the configuration space $\mathbb{R}^{3N}$ and have complicated transformation properties. Furthermore, we show that the expression for T_{intr} given by Rowe and Rosensteel (1979a, b) though having formal validity in classical mechanics, is in fact not valid in a quantum setting.

It is recognised (Gulshani 1977, Buck *et al* 1979) that the difficulties associated with defining a set of intrinsic momenta with well defined action in $\mathbb{R}^{3N}$ is closely related to the fact (Gulshani 1977) that the corresponding intrinsic coordinates do not exist. It is, however, possible to find an appropriate set of $3N$–9 independent intrinsic momenta in some abstract N-dimensional space, as has been shown in a similar context by Ovcharenko (1976). This resolution of the problem uses the fact (Ovcharenko 1976)

† We note that $\bar{J}_{nA}$ are termed 'intrinsic' correctly because they commute with the collective variables I_A, R_{Ai} and Q_{ij} as well as with $\partial/\partial I_A$ in equations (6.5), (6.6) and (6.11) (cf equation (7.6)). In a similar manner $\mathscr{L}_{AB}$ in (7.11) are to be considered intrinsic.

that the generators of the group SO(N) and those of the direct product group SO(N)$\times$SO(N), i.e. the group associated with an N-dimensional asymmetric top (Gulshani 1979), become identical when acting in the factor space SO(N)/SO($N-3$). In the following section we show that T_{intr} can be expressed in terms of a subset of the generators of SO(N)$\times$SO(N) when the action of T_{intr} is restricted to the space of functions defined on the factor space SO(N)/SO($N-3$).

8. Appropriate set of intrinsic momenta

Let us first point out a few important properties of the projector Γ_{nm} in equation (5.9). From equations (7.12), (7.1), (6.5), (5.10) and (5.9) it readily follows that

$$\Gamma_{nm}\bar{R}_{mA} = \bar{R}_{nA} \tag{8.1}$$

$$\bar{R}_{nA}\bar{R}_{nB} = \delta_{AB} \tag{8.2}$$

$$\Gamma_{nm} = \bar{R}_{ni}\bar{R}_{mi} = \bar{R}_{nA}\bar{R}_{mA} \tag{8.3}$$

$$[J_{nm}, \bar{R}_{\tilde{n}A}] = -\mathrm{i}\hbar(\delta_{m\tilde{n}}\bar{R}_{nA} - \delta_{\tilde{n}n}\bar{R}_{mA}). \tag{8.4}$$

Since the $N\times N$ matrix Γ_{nm} is idempotent, i.e. $\Gamma^2=\Gamma$, and has rank three ($=\operatorname{Tr}\Gamma$), three of its eigenvalues are unity and the remaining $N-3$ are zero. It then follows from equations (8.1)–(8.3) that the quantities $\bar{R}_{nA}$ are three ($A=1,2,3$) normalised eigenvectors of Γ_{nm} with eigenvalues unity. The remaining ($N-3$) normalised eigenvectors $\bar{R}_{n\alpha}(\alpha=4,5,\ldots,N)$ of Γ_{nm} with eigenvalues zero and orthogonal to $\bar{R}_{nA}$ can then be defined by

$$\Gamma_{nm}\bar{R}_{n\alpha}\equiv 0 \qquad \bar{R}_{n\alpha}\bar{R}_{n\beta}=\delta_{\alpha\beta} \qquad \bar{R}_{n\alpha}\bar{R}_{nA}=0 \qquad (\alpha,\beta=4,\ldots,N). \tag{8.5}$$

The N eigenvectors $\{\bar{R}_{nA}, \bar{R}_{n\alpha}; A=1,2,3,; \alpha=4\ldots N\}$ may now be regarded as the N columns of $N\times N$ orthogonal matrix $\bar{R}_{n\sigma}(\sigma=1,2,\ldots,N)$ which, of course, diagonalise the $N\times N$ matrix Γ_{nm}. Thus the subscripts $\{\sigma\}\equiv\{A,\alpha\}$ label the N principal axes of Γ†. These axes are connected to the N axes labelled by n by the orthogonal matrix $\bar{R}_{n\sigma}$ in this abstract N-dimensional space, the so called particle-index space (Morinigo 1972, Dzyublik *et al* 1972, Buck *et al* 1979).

The above interpretation allows us to define quantities projected along the three principal axes of Γ labelled by A, thereby simplifying slightly the expression for T_{intr} in equation (7.9). Thus using equation (8.3), we rewrite $\bar{J}_{nA}$ in (7.10) (cf equation (7.3)) in the form

$$\bar{J}_{nA} = J_{An} - \bar{R}_{nB}J_{AB} \tag{8.6}$$

where we have the definitions

$$J_{An}\equiv\bar{R}_{mA}J_{mn} \qquad \mathscr{L}_{AB}\equiv J_{AB}=\bar{R}_{nA}\bar{R}_{mB}J_{nm} \tag{8.7}$$

and where for consistency of notation we have redefined $\mathscr{L}_{AB}$ in (7.11) as J_{AB}. Equations (8.6) and (8.4) then allow us to rewrite T_{intr} in (7.9) as

$$T_{\text{intr}} = \tfrac{1}{2}\sum_{A=1}^{3}\frac{1}{I_A}\left(\sum_{n=1}^{N}J_{An}^2 - \sum_{B=1}^{3}J_{AB}^2\right). \tag{8.8}$$

† From the definition of $\bar{R}_{nA}$ in equation (7.12) we see that if we interpret x_{nA} as three vectors $x^{(A)}$ in N dimensions, then three of these principal axes (those labelled by A) coincide with the orthonormal vectors $(1/\sqrt{I_A})x^{(A)}$.

We note that expression (8.8) involves projections J_{An} and J_{AB} of J_{nm} along different axes (cf the two sets of axes labelled by n and B). However, the number of components of J_{nm} appearing in (8.8) cannot be reduced to $3N-9$ by using the relation $J_{An} \equiv \bar{R}_{n\sigma} J_{A\sigma}$ where $J_{A\sigma}$ are Γ-principal-axes components of J_{nm}. The reason for this is that the $N-3$ columns $\bar{R}_{n\alpha}$ of the $N \times N$ orthogonal matrix $\bar{R}_{n\alpha}$ defined in equations (8.5) do not transform under the action of J_{nm} as columns of an orthogonal matrix, i.e. $[J_{nm}, R_{\tilde{n}\alpha}] \neq -\mathrm{i}\hbar(\delta_{m\tilde{n}}\bar{R}_{n\alpha} - \delta_{n\tilde{n}}\bar{R}_{m\alpha})$. This is in contrast to the transformation properties of the first three columns, $\bar{R}_{nA}$ (cf equation (8.4)). The above assertion is proved in appendix 1. This fact was inadvertently overlooked by Rowe and Rosensteel (1979a, b) in deriving their expression for T_{intr}. Consequently their result for T_{intr} is incorrect, as is shown in appendix 2.

The reason why $\bar{R}_{n\alpha}$ do not transform under J_{nm} as elements of SO(N) is not too surprising: J_{nm} in equation (7.1) are the angular momentum operators, in N-dimensional particle-index space, of the N-point particles whereas the orthogonal matrix $\bar{R}_{n\sigma}$ gives the orientation of the matrix Γ_{nm}, an 'extended' object which may be likened to an N-dimensional asymmetric top. Now, as is well known and as emphasised by Fillipov (1974), there is a difference, even in the three-dimensional space, between the angular momentum operators appropriate for an extended object and those of point particles (see, for example, Gulshani (1979) for the three-dimensional situation). The angular momentum algebra appropriate for an N-dimensional extended object such as Γ_{nm} is that of the direct product group SO(N) $\times$ SO(N) (see, for example, Judd 1975, Gulshani 1979). The corresponding infinitesimal operators of this group are denoted here by the direct sum $\mathrm{so}(N)+\mathrm{so}(N) \equiv \{K_{nm}, K_{\sigma\tilde{\sigma}};\ n, m=1, \ldots, N;\ \sigma, \tilde{\sigma}=1, \ldots, N\}$ where the right-shift operators K_{nm} are chosen to be the $\frac{1}{2}N(N-1)$ angular momentum components along the axes labelled by n and the left-shift operators $K_{\sigma\tilde{\sigma}}$ are those along the principal axes of Γ, i.e. $K_{nm} \equiv \bar{R}_{n\sigma}\bar{R}_{m\tilde{\sigma}}K_{\sigma\tilde{\sigma}}$†.

It is well known that

$$[K_{nm}, \bar{R}_{\tilde{n}\sigma}] = -\mathrm{i}\hbar(\delta_{m\tilde{n}}\bar{R}_{n\sigma} - \delta_{n\tilde{n}}\bar{R}_{m\sigma}) \qquad \text{for all } \sigma \tag{8.9}$$

(cf $[J_{nm}, \bar{R}_{\tilde{n}\alpha}] \neq -\mathrm{i}\hbar(\delta_{m\tilde{n}}R_{n\alpha} - \delta_{n\tilde{n}}\bar{R}_{m\alpha})$) and one can express K_{nm} and $K_{\sigma\tilde{\sigma}}$ in terms of $\frac{1}{2}N^*(N-1)$ Euler angles (Ovcharenko 1976). Similarly, one can express J_{nm} in terms of a subset of these Euler angles. It is also clear that under rotation in this space J_{nm} transforms as an antisymmetric tensor, i.e.

$$[K_{nm}, J_{\tilde{n}\tilde{m}}] = -\mathrm{i}\hbar(\delta_{m\tilde{n}}J_{n\tilde{m}} + \delta_{m\tilde{n}}J_{\tilde{n}n} - \delta_{n\tilde{n}}J_{m\tilde{m}} - \delta_{nm}J_{\tilde{n}m}). \tag{8.10}$$

Furthermore, the operators K_{nm} become identical to J_{nm} when they act on functions Ψ defined on the factor space SO(N)/SO($N-3$) (Ovcharenko 1976), i.e.

$$K_{nm}\Psi(r) \equiv J_{nm}\Psi(r) \qquad r \in \mathrm{SO}(N)/\mathrm{SO}(N-3) \tag{8.11}$$

(cf the three-dimensional case).

Equations (8.11) and (8.9) now allow us to express T_{intr} in (8.8) in terms of only $(3N-9)$ of the operators K_{nm} (and not J_{nm})‡ as follows. Restricting the action of T_{intr} in equation (8.8) to the space of functions $\Psi(r)$ defined on the factor space SO(N)/SO($N-$

† It is observed that K_{nm} and $K_{\sigma\tilde{\sigma}}$ are not defined in the n-particle phase-space in contrast to J_{nm} in equation (7.1). This is because equations (8.5) do not completely determine $\bar{R}_{n\alpha}$ in $\mathbb{R}^{3N}$. A detailed study of the distinction between left and right operators is given by Vanagas (1977).

‡ This is the case in spite of (8.11) because $[J_{nm}, \bar{R}_{\tilde{n}\alpha}]$ can never be equal to $-\mathrm{i}\hbar(\delta_{m\tilde{n}}\bar{R}_{n\alpha} - \delta_{n\tilde{n}}\bar{R}_{m\alpha})$.

3), i.e. $r \in SO(N)/SO(N-3)$, and using equations (8.9), (8.10) and (8.11), one readily obtains the expression

$$
\begin{aligned}
T_{\text{intr}}\Psi(r) &= \tfrac{1}{2}\sum_{A=1}^{3}\frac{1}{I_A}\left(\sum_{n=1}^{N} J_{An}^2 - \sum_{B=1}^{3} J_{AB}^2\right)\Psi(r) \\
&= \tfrac{1}{2}\sum_{A=1}^{3}\frac{1}{I_A}\left(\sum_{\sigma=1}^{N} K_{A\sigma}^2 - \sum_{B=1}^{3} K_{AB}^2\right)\Psi(r) \\
&= \tfrac{1}{2}\sum_{A=1}^{3}\sum_{\alpha=4}^{N}\frac{1}{I_A}K_{A\alpha}^2\ \Psi(r)
\end{aligned}
\tag{8.12}
$$

with $r \in SO(N)/SO(N-3)$, $K_{A\alpha} \equiv \bar{R}_{nA}\bar{R}_{m\alpha}K_{nm}$ and $K_{AB} \equiv \bar{R}_{nA}\bar{R}_{mB}K_{nm}$. It is observed that only $3N-9$ operators $K_{A\alpha}$ appear in equation (8.12). These are the appropriate intrinsic momenta we have been seeking, but it must be emphasised that they are appropriate only in the space $\Psi(r)$. Combining equations (8.12) and (6.8) (cf (6.2)), we finally obtain, for the transformed N-particle kinetic energy, the expression

$$
\begin{aligned}
T\Psi(r) = \Bigg\{ &\tfrac{1}{2}\sum_{A=1}^{3}\sum_{\alpha=4}^{N}\frac{1}{I_A}K_{A\alpha}^2 - 2\hbar^2\sum_{A=1}^{3} I_A\left[\frac{\partial^2}{\partial I_A^2} + \left(\frac{N-2}{2I_A} + \sum_{B\neq A}^{3}\frac{1}{I_A - I_B}\right)\frac{\partial}{\partial I_A}\right] \\
&+ \tfrac{1}{2}\sum_{A<B}^{3}\left(\frac{I_A + I_B}{(I_A - I_B)^2}(L_{AB}^2 + K_{AB}^2) - \frac{4(I_A I_B)^{1/2}}{(I_A - I_B)^2}L_{AB}K_{AB}\right)\Bigg\}\Psi(r)
\end{aligned}
\tag{8.14}
$$

where we have also replaced $\mathscr{L}_{AB}$ by K_{AB} (cf equations (6.8*c*), (7.11) and (8.7)). Equation (8.14) is seen to be identical to that given by Dzyublik *et al* (1972), Fillipov (1974), Ovcharenko (1976) and Vanagas (1977).

An appropriate irreducible basis set for solving the Schrödinger equation with the kinetic energy (8.14) has been studied in great detail by many authors (Vanagas and Kalinauskas 1974, Fillipov 1974, Petrauskas and Sabalyauskas 1975, Asherova *et al* 1976, Vanagus 1976) and we will not discuss these in this paper. However, the goal of such studies is to put the phenomenological collective model of Bohr (Bohr 1952, Bohr and Mottelson 1953) on a microscopic basis by finding an appropriate decomposition of the N-particle Hilbert space into collective and intrinsic parts with small coupling between them. In equation (8.14) we see that such a coupling is mediated by K_{AB}. However, there is also a dynamical type of coupling arising from the particle interactions which has not been discussed in his paper. How to deal with these questions is still not completely resolved. In a forthcoming publication we will consider some questions related to the effects of the collective motions described in equation (8.14) on the intrinsic structure.

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Appendix 1

Here we show that the $N-3$ columns $\bar{R}_{n\alpha}$ $(\alpha = 4, \ldots, N)$ of the $N \times N$ orthogonal matrix $\bar{R}_{n\sigma}$ $(\sigma = 1, \ldots, N)$ defined in equations (8.5) do not transform under J_{nm} as the first three columns $\bar{R}_{nA}$ ($A=1,2,3$), i.e. as in equation (8.4). The proof is as follows. Suppose $\bar{R}_{n\alpha}$ did transform according to

$$[J_{nm}, \bar{R}_{\tilde{n}\alpha}] = -i\hbar(\delta_{m\tilde{n}}\bar{R}_{n\alpha} - \delta_{n\tilde{n}}\bar{R}_{m\alpha}). \qquad \text{(A1.1)}$$

Then multiplying (A1.1) from the left by $\bar{R}_{n\beta}$ and $\bar{R}_{m\gamma}$, summing over n and m and using the orthogonality relation $\bar{R}_{n\alpha}\bar{R}_{n\beta} = \delta_{\alpha\beta}$ in (8.5), we obtain

$$[J_{\beta\gamma}, \bar{R}_{\tilde{n}\alpha}] = -i\hbar(\delta_{\alpha\beta}\bar{R}_{n\gamma} - \delta_{\alpha\gamma}\bar{R}_{n\beta}) \qquad \text{(A1.2)}$$

where the left-shift operators $J_{\beta\gamma} \equiv \bar{R}_{n\beta}\bar{R}_{m\gamma}J_{nm}$. But from the definition of $\bar{R}_{nA}$ in (7.12) and the orthogonality relation $\bar{R}_{nA}\bar{R}_{n\alpha} = 0$ in (8.5) we have

$$\bar{R}_{n\alpha}x_{nA} = 0 \qquad \text{for all } \alpha \text{ and } A \qquad \text{(A1.3)}$$

and consequently

$$J_{\beta\gamma} \equiv \bar{R}_{n\beta}\bar{R}_{m\gamma}J_{nm} \equiv 0 \qquad \text{(A1.4)}$$

(cf equation (7.1))†. Equations (A1.4) and (A1.2) then imply that $\bar{R}_{n\alpha} = 0$ for all n and α. But this is not possible (cf equations (8.5)). We must, therefore, conclude that equation (A1.2) is false.

Appendix 2

Rowe and Rosensteel (1979a, b) define the $3N$–9 intrinsic momenta $\mathscr{I}_{\alpha A} \equiv \bar{R}_{n\alpha}\bar{R}_{mA}J_{nm}$ and derive the expression

$$T_{\text{intr}}^{(\text{RR})} = \frac{1}{2m}\sum_{A=1}^{3}\sum_{\alpha=4}^{N}\frac{1}{I_A}\mathscr{I}_{\alpha A}^2$$

for the intrinsic kinetic energy based on the assumption that the quantity

$$Z_{\alpha A} \equiv \sum_{\substack{m=1\\ n-1}}^{N}\sum_{j=1}^{3}\frac{\partial}{\partial x_{mj}}(\bar{R}_{m\alpha}\bar{R}_{nA}x_{nj})$$

vanishes (see Rowe and Rosensteel 1979a, equations (26) and (29)). We note first that the momenta $\mathscr{I}_{\alpha A}$ are not well defined in the phase-space because $\bar{R}_{n\alpha}$ are not defined in $\mathbb{R}^{3N}$, as has been pointed out earlier. Secondly, one can show that $Z_{\alpha A}$ cannot vanish so that the expression for $T_{\text{intr}}^{(\text{RR})}$ is not correct. The non-vanishing of $Z_{\alpha A}$ can be seen as follows. Since $\bar{R}_{m\alpha}\bar{R}_{mA} = \bar{R}_{m\alpha}x_{mj} = 0$ (cf equation (A1.3)), one can rewrite $Z_{\alpha A}$ as

$$\begin{aligned} Z_{\alpha A} &\equiv \frac{\partial}{\partial x_{mj}}(\bar{R}_{m\alpha}\bar{R}_{nA}x_{nj}) - \frac{\partial}{\partial x_{nj}}(\bar{R}_{m\alpha}\bar{R}_{nA}x_{mj}) \\ &\equiv \bar{R}_{nA}J_{nm}(\bar{R}_{m\alpha}) \end{aligned} \qquad \text{(A2.1)}$$

where equation (8.4) has been used. Now the RHS of equation (A1.5) would vanish if equation (A1.1) were valid. In fact, Rowe and Rosensteel (1979b) assumed equation (A1.1) to be valid and used it to show that $Z_{\alpha A}$ vanishes, thereby deriving their result for $T^{(\text{RR})}$. We know now that equation (A1.1) is not valid. Moreover, one can easily and explicitly show that in the special case of three dimensions the RHS of equation (A2.1)

† Note that (A1.4) is merely a generalisation of the situation in three dimensions where the component of the angular momentum along the particle radius vector vanishes.

does not vanish. In this special case J_{nm} becomes identical to the three components of the physical angular momentum of the particles which are expressible in terms of the polar angles. $\bar{R}_{nA}$ and $\bar{R}_{m\alpha}$ are likewise identifiable with the first and the remaining two columns of the 3×3 rotation matrix expressible in terms of the usual Euler angles (Rose 1957).

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