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Geometry of collective motions

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Abstract. A general projection method for decomposing the kinetic energy of an N-particle system into collective and intrinsic parts defined respectively on the orbits and the orbit space of a Lie transformation group is given. Specific targets of the application of the method are the kinematical group $GL^+(3, \mathbb{R})$ and the quotient set $GL^+(3, \mathbb{R})/SO(3)$ for their importance in microscopic formulation of nuclear collective motions. For these two cases the orbit spaces in the particle configuration space are shown to be identifiable with the Grassman and Stiefel manifolds of 3-planes and 3-frames respectively. Some problems related to expressing the kinetic energy in terms of vector fields on these manifolds are resolved. In particular, non-integrable coordinates previously used by one of the present authors is shown to arise from the imposition of unacceptable conditions. Finally we consider the corresponding decomposition of the N-particle Hilbert space. It is proposed that an appropriate basis function for the $GL^+(3, \mathbb{R})$ collective model is provided by an irreducible representation of the boson SU(6) group.

1. Introduction

The phenomenological nuclear collective models of Bohr-Mottelson (Bohr 1952, Bohr and Mottelson 1953, 1975, Bohr *et al* 1976) have had considerable success in accounting for various rotational and vibrational features in certain nuclei. In attempts to formulate these models microscopically many authors have adopted a geometric viewpoint. The objective in this approach is to extract the model Hamiltonian by using a Lie transformation group to effect a change of coordinates on the *N*-particle configuration space \mathbb{R}^{3N} from the particle to a set of collective and intrinsic coordinates. The resulting decomposition of the total particle kinetic energy into collective and intrinsic parts then defines the model kinetic energy. The collective potential energy will then have to be obtained from other considerations.

To describe the rotational motion Bohr (1954), Villars (1957), Scheid and Greiner (1968), Villars and Cooper (1970) and Rowe (1970) used orbits of the kinematical group SO(3) as the collective submanifold of \mathbb{R}^{3N} . This work was later generalised independently by many authors to the simpler and physically more interesting case of the coupled rotation-vibrational motion by using the groups GL⁺(3, \mathbb{R}) (Cusson 1968, Gulshani and Rowe 1976, Gulshani 1977, 1978, Buck *et al* 1979) and SL(3, \mathbb{R}) (Ogura 1973, Weaver *et al* 1976) and the quotient set GL⁺(3, \mathbb{R})/SO(3) (Zickendraht 1971, Dzyublik *et al* 1972, Morinigo 1972, 1974, Filippov 1974, Ovcharenko 1976, Vanagas 1977). Although the final results of these GL⁺(3, \mathbb{R}) transformations are similar, different authors have used different decompositions of \mathbb{R}^{3N} and different decompositions of the tangent space to \mathbb{R}^{3N} , i.e. the particle momentum space.

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Recently projection operators for the Lie algebras so(3) and $gl(3, \mathbb{R})$ were given and it was shown (Gulshani 1981) that these operators provide a simple and a transparent means of effecting the decomposition of the particle momenta and the total kinetic energy. The purpose of this paper is firstly to generalise this projection method to an arbitrary Lie group using some elementary concepts in differential geometry; and secondly to rederive the $GL^+(3, \mathbb{R})$ results in this general framework[†] and analyse carefully the various problems raised in the previous paper. In § 2 we review briefly the geometric method of constructing collective and intrinsic submanifolds of \mathbb{R}^{3N} and vector fields on them. These manifolds are identified respectively with the orbits and the orbit space of a Lie transformation group modulo an isotropy subgroup H. The decomposition of the tangent space to \mathbb{R}^{3N} into subspaces tangent and normal to the collective submanifold using a projector operator is then carried out in § 3. The corresponding decomposition for the total particle kinetic energy is then obtained. In this section we also discuss various other possible decompositions.

In § 4 these results are specialised to $GL^+(3, \mathbb{R})/H$. In § 4.1 it is shown that, with H = e, the identity element in $GL^+(3, \mathbb{R})$ and H = SO(3), the intrinsic submanifold of R^{3N} is identifiable respectively with the Grassman manifold of 3-planes and the Stiefel manifold of 3-frames in \mathbb{R}^N . In § 4.2 the $gl(3, \mathbb{R})$ projector is constructed and the decompositions of the particle momenta and the total kinetic energy into collective and intrinsic parts with respect to the different sets of collective coordinates are derived. Different sets of basis functions for the diagonalisation of the collective Hamiltonian are discussed. In particular it is suggested that irreducible representations of SU(6), employed in the interacting boson model of Arima and Iachello, provide suitable basis functions for the GL*(3, \mathbb{R}) collective model considered here. Finally in § 4.3 we use diffeomorphisms between the Grassman and the Stiefel manifolds and quotient spaces of SO(N) to express the intrinsic kinetic energy in terms of vector fields on SO(N). Some problems related to doing this are resolved. In particular it is shown that non-integrable coordinates used previously arise from imposing incompatible constraints.

2. Lie transformation groups and collective-intrinsic submanifolds of \mathbb{R}^{3N}

The configuration of a system of N discrete particles in the three-dimensional physical space is given by a point in the 3N-dimensional Euclidean space \mathbb{R}^{3N} , known as the configuration space. \mathbb{R}^{3N} is a manifold as well as a vector space of dimension 3N. A natural (global) coordinate system (atlas of charts) on \mathbb{R}^{3N} is commonly chosen to be the rectangular Cartesian coordinates $\{x^{ni}; i = 1, 2, 3; 1 \le n \le N\}$. The particle momenta $p_{ni} \equiv -i\hbar(\partial/\partial x^{ni})$ are (tangent) vector fields on \mathbb{R}^{3N} and the set $\{\partial/\partial x^{ni}\}$ span, at each point $x \in \mathbb{R}^{3N}$, the 3N-dimensional tangent vector space $T_x \mathbb{R}^{3N}$ to \mathbb{R}^{3N} . \mathbb{R}^{3N} is a flat Riemannian manifold with the Riemannian metric g defined by the usual Euclidean inner product (see, among others, Brickell and Clark 1970, p 161, Matsushima 1972, p 40, Boothby 1975, p 184)

$$g_{ni,mj} \equiv g\left(\frac{\partial}{\partial x^{ni}}, \frac{\partial}{\partial x^{ni}}\right) = \delta_{nm}\delta_{ij}.$$
(2.1)

⁺ Recently Guillemin and Sternberg (1980) have given the problem of collective motion a mathematical exposition in the framework of the momentum map.

The total kinetic energy of the system is then given by the Laplacian

$$T = \frac{1}{2M} \sum_{n=1}^{N} \sum_{i=1}^{3} p_{ni}^{2}$$
(2.2)

where M is the mass of each particle[†].

The attempt in the geometric approach to realising collective models microscopically is to seek an appropriate direct-product decomposition $\mathbb{R}^{3N} = \mathcal{M}_G \times \mathcal{M}_{intr}$ of \mathbb{R}^{3N} into collective, \mathcal{M}_G , and intrinsic, \mathcal{M}_{intr} , submanifolds. The corresponding direct-sum decomposition

$$T_{\mathbf{x}} \mathbb{R}^{3N} = T_{\mathbf{x}} \mathcal{M}_{\mathbf{G}} \oplus (T_{\mathbf{x}} \mathcal{M}_{\mathbf{G}})^{c}$$
(2.3)

$$p_{ni} = p_{ni}^{\text{coll}} + p_{ni}^{\text{intr}} \tag{2.4}$$

(where $T_x \mathcal{M}_G$ is the tangent space to \mathcal{M}_G spanned by some (collective) vector fields given below and $(T_x \mathcal{M}_G)^c$ is the vector space complement) then defines the decomposition of Tin (2.2) into collective and intrinsic parts. The expressions obtained for these separate parts is observed to depend crucially on the choice of $(T_x \mathcal{M}_G)^c$. This choice can be made in a number of ways. For example, we may set $(T_x \mathcal{M}_G)^c = T_x \mathcal{M}_{intr}$ in which case p_{ni}^{intr} are vector fields on \mathcal{M}_{intr} . In this paper we choose it to be the normal space to \mathcal{M}_G , i.e. we set $(T_x \mathcal{M}_G)^c = (T_x \mathcal{M}_G)^{\perp}$, the orthogonal complement of $T_x \mathcal{M}_G$ in $T_x \mathbb{R}^{3N}$. In this case p_{ni}^{intr} are vector fields along \mathcal{M}_{intr} but not necessarily on \mathcal{M}_{intr} because, in general, $(T_x \mathcal{M}_G)^{\perp} \neq$ $T_x \mathcal{M}_{intr}$ as we shall see in § 4.3. This choice has the advantage that the resulting orthogonality‡

$$g(p_{ni}^{\text{coll}}, p_{mj}^{\text{intr}}) = 0, \qquad (2.5)$$

with g as in (2.1), simplifies the decomposition of the kinetic energy T in (2.2). For then one readily obtains the result (see § 3)

$$T = T_{\rm coll} + T_{\rm intr} \tag{2.6}$$

with no cross terms between the collective, T_{coll} , and intrinsic, T_{intr} , parts of T. We shall be working in the basis sets $\{x^{ni}\}$ and $\{\partial/\partial x^{ni}\}$ for convenience and to ensure that all functions and vector fields used are well defined on \mathbb{R}^{3N} .

Now a natural way of realising collective, \mathcal{M}_G , and intrinsic, \mathcal{M}_{intr} , submanifolds of \mathbb{R}^{3N} is to identify them with the orbits and the orbit space respectively of a Lie group which acts on \mathbb{R}^{3N} as a Lie transformation group§. Let us now briefly review some aspects of the action of a Lie transformation group on a manifold such as $\mathbb{R}^{3N} \parallel$.

A Lie group G acts on \mathbb{R}^{3N} (on the left) as a Lie transformation group when one is given a mapping

$$\Phi: \mathbf{G} \times \mathbb{R}^{3N} \to \mathbb{R}^{3N}, \qquad x = \Phi(g, \bar{x})$$
(2.7)

[†] Note that (2.2) is equivalent to the so-called Laplace–Beltrami operator by virtue of the flatness of \mathbb{R}^{3N} (cf (2.1)) (see, for example, Hermann 1968, Gulshani and Rowe 1976, appendix I).

[‡] This orthogonality was first pointed out and used in this context by one of the present authors (Gulshani and Rowe 1976, appendix III, Gulshani 1977).

§ This geometric approach is to be compared with the method of spectrum generating algebras (Dashen and Gell-Mann 1965, Dothan *et al* 1965, Ui 1970, Hermann 1972, Weaver and Biedenharn 1972, Weaver *et al* 1973, 1976, Gulshani and Rowe 1976) and of dynamical groups (Dyson 1966, Arima and Iachello 1975, 1976, 1978, Dzholos *et al* 1976, Iachello 1979).

|| For more detail refer to, among others, Auslander and Mackenzie (1963), Tondeur (1969), Brickell and Clark (1970), Warner (1971), Matsushima (1972), Sagle and Walde (1973) and Boothby (1975).

for $\bar{x} \in \mathbb{R}^{3N}$, $g \in G$ and some $x \in \mathbb{R}^{3N}$, such that, for $g_1, g_2 \in G$, $\Phi(g_1, \Phi(g_2, \bar{x})) = \Phi(g_1g_2, \bar{x})$ and, for the identity element $e \in G$, $\Phi(e, \bar{x}) = \bar{x}$. The set of points $\{x = \Phi(g, \bar{x}) | x \in \mathbb{R}^{3N}$, all $g \in G$ } is a subset of \mathbb{R}^{3N} called the orbit of \bar{x} under the (left) action of G. The action of G in (2.7) is said to be effective if the identity $e \in G$ is the only element for which $\Phi(g, \bar{x}) = \bar{x}$. In general G does not act effectively and one may then find (at each point \bar{x}) a subgroup H of G for which \bar{x} is a fixed point, i.e. $\Phi(h, \bar{x}) = \bar{x}$ for all $h \in H$. The subgroup H is called the stability or the isotropy subgroup of G at \bar{x} . If H is a closed (Lie) group, then the set of all left cosets $G/H = \{gH|g \in G\}$ is a C^{∞} manifold of dimension given by dim(G/H) = dim G - dim H. G/H is called the quotient manifold, the coset or the factor space[†]. Evidently G/H acts effectively on \mathbb{R}^{3N} .

One can now prove the following theorem (Brickell and Clark 1970, p 250): Let G be a Lie transformation group of \mathbb{R}^{3N} and H the isotropy closed subgroup at the point $\bar{x} \in \mathbb{R}^{3N}$. Then the C^{∞} injective mapping

$$\psi_{\bar{x}} \colon G/H \to \mathbb{R}^{3N},\tag{2.8}$$

defined by

$$x \equiv \psi_{\bar{x}}(gH) \equiv \Phi(gH, \bar{x}) = \Phi(g, \Phi(H, \bar{x})) = \Phi(g, \bar{x})$$

where Φ is as in (2.7), is an imbedding of the quotient manifold G/H into \mathbb{R}^{3N} . In other words, each orbit $\mathcal{M}_{G/H} \equiv \{x = \Phi(gH, \bar{x}) | g \in G\}$ of \bar{x} is a submanifold of \mathbb{R}^{3N} diffeomorphic to G/H. The diffeomorphism in (2.8) sets up an isomorphism between the tangent spaces $T_c(G/H)$ and $T_x \mathcal{M}_{G/H}$ to G/H and the orbit $\mathcal{M}_{G/H}$ at each pair points $c \equiv gH$ and $x = \psi_{\bar{x}}(gH)$. The imbedding, on the other hand, ensures that $T_x \mathcal{M}_{G/H}$ is a subspace of $T_x \mathbb{R}^{3N}$. The correspondence between vector fields on G/H and $\mathcal{M}_{G/H}$ is given by the injective mapping (the differential of $\psi_{\bar{x}}$)

$$\psi_{\hat{s}}^*: T_0(G/H) \to T_x \mathcal{M}_{G/H}$$
(2.9)

where $0 \equiv e H = H$ is the identity element in G/H. $\psi_{\bar{x}}^*$ in (2.9) is defined as follows: for every tangent vector $Y_0 \in T_0(G/H)$ and any C^{∞} real-valued function f on G/H we have $\psi_{\bar{x}}^*(Y_0) \in T_x \mathcal{M}_{G/H}$ and $\psi_{\bar{x}}^*(Y_0)(f) \equiv Y_0(f \circ \psi_{\bar{x}})$. More specifically, let r be the dimension of G/H and (y^1, \ldots, y') a set of coordinate functions on G/H so that the r tangent vectors $\{(\partial/\partial y^{\alpha})_0 | 1 \leq \alpha \leq r\}$ span $T_0(G/H)$. Then the tangent vectors $(X_{\alpha})_x \in T_x \mathcal{M}_{G/H}$, corresponding to $(\partial/\partial y^{\alpha})_0$ and expanded in the basis vectors $\{(\partial/\partial x^{ni})_x\}$ of $T_x \mathbb{R}^{3N}$, are given by[‡]

$$(X_{\alpha})_{x} \equiv \psi_{\bar{x}}^{*} \left(\frac{\partial}{\partial y^{\alpha}}\right)_{0} = \left[\frac{\partial}{\partial y^{\alpha}} \left(x^{ni} \circ \psi_{\bar{x}}(g\mathbf{H})\right)\right]_{0} \left(\frac{\partial}{\partial x^{ni}}\right)_{x}$$
$$\equiv X_{\alpha}^{ni}(x) \left(\frac{\partial}{\partial x^{ni}}\right)_{x} \qquad 1 \le \alpha \le r$$
(2.10)

where the expression in the square bracket is to be evaluated at the identity element 0 after the indicated differentiation. The set of tangent vectors $\{(X_{\alpha})_x | 1 \le \alpha \le r\}$ clearly spans $T_x \mathcal{M}_{G/H}$ as $\psi_{\bar{x}}^*$ is an injection.

Finally, we observe that $T_x \mathcal{M}_{G/H}$ and the quotient vector space $\mathcal{A}_G/\mathcal{A}_H$, where \mathcal{A}_G and \mathcal{A}_H are respectively the Lie algebras of G and H, are isomorphic. This follows immediately from the natural isomorphism that exists between $\mathcal{A}_G/\mathcal{A}_H$ and $T_0(G/H)$

 $^{^{+}}$ G/H is a homogeneous space of G since G acts transitively on G/H. A transitive action is one for which any two elements of the set can be connected by some element of G.

[‡] Summation over repeated indices is assumed throughout.

(Matsushima 1972, p 236)[†]. These isomorphisms arise in a simple way. The Lie algebra \mathcal{A}_G of G is defined as the set of all left-invariant vector fields on G which are determined uniquely by their values at $e \in G$ by left translations (Brickell and Clark 1970, p 218, Matsushima 1972, p 188, Boothby 1975, pp 119, 154). One thereby arrives at the isomorphism between \mathcal{A}_G and $T_e G$. On the other hand, when the isotropy subgroup H is the identity $e \in G$, one can show (Brickell and Clark 1970, pp 244, 248, Matsushima 1972, p 236) that the set of vector fields X_{α} in (2.10) induced on \mathcal{M}_G form a Lie algebra \mathcal{R}_G isomorphic to the Lie algebra of right-invariant vector fields on G. Again these right-invariant vector fields are determined uniquely by their values at $e \in G$ by right translations. The basis vectors of \mathcal{A}_G and \mathcal{R}_G are often called the infinitesimal generators and operators of G respectively. When $H \neq e$, the above isomorphisms still exist but the left- and right-invariant vector fields on G/H do not because G/H is not a group unless H is a normal (invariant) subgroup.

We now define a collective submanifold of \mathbb{R}^{3N} to be the orbits $\mathcal{M}_{G/H}$ of G/H. The collective coordinates and vector fields are then given respectively by a set of appropriate coordinate functions $\{y^{\alpha} | 1 \leq \alpha \leq r\}$ on G/H and the corresponding vector fields X_{α} in (2.10) on $\mathcal{M}_{G/H}$. The intrinsic submanifold \mathcal{M}_{intr} , which complements $\mathcal{M}_{G/H}$ in the direct-product decomposition $\mathbb{R}^{3N} = \mathcal{M}_{G/H} \times \mathcal{M}_{intr}$, is then naturally identified with a quotient space of \mathbb{R}^{3N} as follows. The action of G defines an equivalence relation on \mathbb{R}^{3N} : each x in (2.7) is equivalent to \bar{x} and, hence, \bar{x} determines an equivalence class. Thus an orbit of G is an equivalence class. The set of all equivalence classes of G in \mathbb{R}^{3N} is a quotient space called the orbit space of G and denoted by \mathbb{R}^{3N}/G (Brickell and Clark 1970, pp 91, 97, Boothby 1975, pp 60, 93). \mathcal{M}_{intr} is, therefore, naturally identifiable with the orbit space \mathbb{R}^{3N}/G of G. Thus, if $\{\xi^{\sigma} | 1 \leq \sigma \leq 3N - r\}$ is an appropriate set of (intrinsic) coordinates on $\mathcal{M}_{intr} = \mathbb{R}^{3N}/G$, each orbit (2.7) of G may be parametrised according to

$$x = \Phi(\tilde{g}(y^{\alpha}), \bar{x}(\xi^{\alpha})), \qquad \tilde{g} \in G/H, \qquad \bar{x} \in \mathcal{M}_{intr}.$$
(2.11)

The intrinsic vector fields are then given by vector fields on \mathcal{M}_{intr} .

3. Decomposition of momenta and kinetic energy

We now seek a decomposition of the particle momenta p_{ni} and the total kinetic energy T in (2.2) into collective and intrinsic parts and expressed in terms of the r collective vector fields X_{α} in (2.10) on $\mathcal{M}_{G/H}$ and some convenient set of intrinsic vector fields on \mathcal{M}_{intr} . As was explained in § 2, it is convenient, for this purpose, to choose the direct-sum decomposition[‡]

$$T_{x}\mathbb{R}^{3N} = T_{x}\mathcal{M}_{G/H} \oplus (T_{x}\mathcal{M}_{G/H})^{\perp}$$
(3.1)

where $(T_x \mathcal{M}_{G/H}^{\perp})$ is the (3N-r)-dimensional orthogonal vector space complement of $T_x \mathcal{M}_{G/H}$ in $T_x \mathbb{R}^{3N}$, i.e. the normal space to $\mathcal{M}_{G/H}$. According to the procedure given previously (Gulshani 1981) the decomposition (3.1) is accomplished simply in terms of

 \ddagger Observe that, in general, $(T_x \mathcal{M}_{G/H})^{\perp} \neq T_x \mathcal{M}_{intr}$, i.e. \mathcal{M}_{intr} is not an integral manifold of the distribution determined by the normal space $(T_x \mathcal{M}_{G/H})^{\perp}$ (cf § 4.3).

[†] From a general theorem on vector spaces (Hoffman and Kunze 1961, p 323) one knows that the quotient space $\mathcal{A}_G/\mathcal{A}_H$ is isomorphic to any subspace complement of \mathcal{A}_H in \mathcal{A}_G , i.e. $\mathcal{A}_G = \mathcal{A}_H \oplus (\mathcal{A}_G/\mathcal{A}_H)$ (see also Sagle and Walde 1973, p 151).

the projection operator Γ on $T_x \mathcal{M}_{G/H}$

$$\Gamma: T_x \mathbb{R}^{3N} \to T_x \mathcal{M}_{G/H}$$
(3.2)

as follows. Since $\mathcal{M}_{G/H}$ is a submanifold of \mathbb{R}^{3N} , the Riemannian metric g on \mathbb{R}^{3N} in (2.1) induces a metric h on $\mathcal{M}_{G/H}$ defined by

$$h_{\alpha\beta} \equiv g(X_{\alpha}, X_{\beta}) = X_{\alpha}^{ni} X_{\beta}^{mj} g_{ni,mj} = X_{\alpha}^{ni} X_{\beta}^{ni} \qquad 1 \le \alpha, \beta \le r$$
(3.3)

where X_{α}^{ni} are defined in (2.10). If the metric tensor *h* is non-degenerate, the matrix representation of the projection operator Γ in (3.2) with respect to the basis $\{\partial/\partial x^{ni}\}$ for $T_x \mathbb{R}^{3N}$ is then readily constructed (cf Hoffman and Kunze 1961, p 232, Gulshani 1981). One obtains

$$\Gamma_{ni,mj} \equiv X_{\alpha}^{ni} h^{\alpha\beta} X_{\beta}^{mj} \qquad 1 \le \alpha, \beta \le r$$
(3.4)

where the inverse metric tensor $h^{\alpha\beta}$ is defined by $h^{\alpha\gamma}h_{\gamma\beta} \equiv \delta^{\alpha}_{\beta}$. From the definition (3.4) it is easy to show that Γ meets all the requirements of the projector (3.2): Γ is symmetric, i.e. $\Gamma_{ni,mj} = \Gamma_{mj,ni}^{\dagger}$, and idempotent, i.e.

$$\Gamma_{ni,mj}^2 = \Gamma_{ni,\bar{n}k} \Gamma_{\bar{n}k,mj} = \Gamma_{ni,mj}$$
(3.5)

and

$$\Gamma_{ni,mj} \boldsymbol{X}_{\alpha}^{mj} = \boldsymbol{X}_{\alpha}^{ni}. \tag{3.6}$$

 Γ effects the projection in (3.2) according to

$$\Gamma\left(\frac{\partial}{\partial x^{ni}}\right) \equiv \Gamma_{ni,mj} \frac{\partial}{\partial x^{mj}} = X^{ni}_{\alpha} h^{\alpha\beta} X_{\beta}$$
(3.7)

where definitions (2.10) and (3.4) have been used. When evaluated at point x, the right-hand side of (3.7) is clearly a vector in $T_x \mathcal{M}_{G/H}$. Defining the action of Γ on X_{α} in (2.10) by

$$\Gamma(X_{\alpha}) \equiv X_{\alpha}^{ni} \Gamma\left(\frac{\partial}{\partial x^{ni}}\right)$$
(3.8)

we observe from (3.7) that (cf (3.6))

$$\Gamma(\boldsymbol{X}_{\alpha}) = \boldsymbol{X}_{\alpha}.$$
(3.9)

This shows that Γ acts in $T_{x}\mathcal{M}_{G/H}$ as a unit operator. Since Γ is idempotent, rank $\Gamma = \operatorname{Tr} \Gamma = \sum_{ni} \Gamma_{ni,ni} = \sum_{\alpha=1}^{r} 1 = r = \dim \mathcal{M}_{G/H} = \dim(T_{x}\mathcal{M}_{G/H})$. Thus the mapping in (3.2) is onto.

The decomposition (3.1) is then given simply by[‡]

$$p_{ni} \equiv -i\hbar \frac{\partial}{\partial x^{ni}} = \Gamma_{ni,mj} p_{mj} + \Lambda_{ni,mj} p_{mj}$$

$$= -i\hbar X_{ni}^{ni} \hbar^{\alpha\beta} X_{\beta} + \Lambda_{ni,mj} p_{mj} \qquad 1 \le \alpha, \beta \le r \qquad (3.10)$$

$$\equiv p_{ni}^{\text{coll}} + p_{ni}^{\text{intr}}$$

⁺ This property is evidently important since otherwise Γ is only left or right idempotent. The order of multiplication then becomes a problem. An example of this situation arises in the construction of a projection operator for linear irrotational flow.

[‡] Note that combinations of different projectors (see, for example, Pease 1965) may be used to effect a simultaneous decomposition of the space into different collective subspaces, as for example, into centre-of-mass and other collective spaces (cf appendix 2).

where (3.7) has been used and

$$\Lambda_{ni,mj} \equiv \delta_{nm} \delta_{ij} - \Gamma_{ni,mj}. \tag{3.11}$$

Clearly $(T_x \mathcal{M}_{G/H})^{\perp}$ is the null space of Γ and Λ projects $T_x \mathbb{R}^{3N}$ onto $(T_x \mathcal{M}_{G/H})^{\perp}$ along $T_x \mathcal{M}_{G/H}$. From the relation

$$\Gamma_{ni,\bar{m}k}\Lambda_{\bar{m}k,mj} = 0 \tag{3.12}$$

(cf (3.5)) it follows that equation (3.10) gives the decomposition of the particle momenta p_{ni} into mutually orthogonal collective, p_{ni}^{coll} , and intrinsic, p_{ni}^{intr} , parts, i.e. $g(p_{ni}^{coll}, p_{nj}^{intr}) = 0$. The second line in (3.10) gives the expression for p_{ni}^{coll} in terms of the collective vector fields X_{α} .

In squaring (3.10) to obtain the corresponding decomposition of the total particle kinetic energy (2.2) into collective and intrinsic parts, it is important to note that $\Gamma_{ni,mj}$ are C^{∞} real-valued functions on \mathbb{R}^{3N} . Thus Γ and $\partial/\partial x^{ni}$ and hence p_{ni}^{coll} and p_{ni}^{intr} do not commute. However, a simple rearrangement of terms, using commutators, yields

$$T = \frac{1}{2M} \sum_{ni} p_{ni}^2 = \frac{1}{2M} p_{ni} \Gamma_{ni,mj} p_{mj} + \frac{1}{2M} p_{ni} \Lambda_{ni,mj} p_{mj} = T_{\text{coll}} + T_{\text{intr.}}$$
(3.13)

We may now use (3.7) to express the collective kinetic energy T_{coll} in terms of the collective vector fields X_{α} :

$$T_{\text{coll}} = \frac{1}{2M} p_{ni} \Gamma_{ni,mj} p_{mj} = -\frac{\hbar^2}{2M} X_{\alpha} h^{\alpha\beta} X_{\beta} - \frac{\hbar^2}{2M} \left(\frac{\partial}{\partial x^{ni}} X_{\alpha}^{ni} \right) h^{\alpha\beta} X_{\beta} \qquad 1 \le \alpha, \beta \le r.$$
(3.14)

In connection with the definitions of T_{coll} and T_{intr} in (3.13) it is observed from (3.10) that

$$T_{\rm coll} = \frac{1}{2M} \sum_{ni} (p_{ni}^{\rm coll})^2 + \frac{1}{2M} \sum_{ni} p_{ni}^{\rm intr} p_{ni}^{\rm coll}$$

and

$$T_{\rm intr} = \frac{1}{2M} \sum_{ni} (p_{ni}^{\rm intr})^2 + \frac{1}{2M} \sum_{ni} p_{ni}^{\rm coll} p_{ni}^{\rm intr}.$$

Thus, in general,

$$T_{\text{coll}} \neq \frac{1}{2M} \sum_{ni} (p_{ni}^{\text{coll}})^2$$
 and $T_{\text{intr}} \neq \frac{1}{2M} \sum_{ni} (p_{ni}^{\text{intr}})^2$

as might be expected from the decomposition (3.10) because, in general,

$$\sum_{ni} p_{ni}^{\text{coll}} p_{ni}^{\text{intr}} \neq 0 \neq \sum_{ni} p_{ni}^{\text{intr}} p_{ni}^{\text{coll}}$$

in spite of the orthogonality $g(p_{ni}^{\text{coll}}, p_{mj}^{\text{intr}}) = 0$ (cf § 4.2 and appendix 2).

Let us now consider T_{intr} in (3.13). In spite of the absence of any apparent coupling terms in (3.13), one expects T_{coll} and T_{intr} to be somehow coupled. To reveal this coupling and to facilitate other physical considerations it is desirable to seek a complete set of vector fields $\{Z_{\nu}|1 \le \nu \le 3N-4\}$ on \mathcal{M}_{intr} and express T_{intr} in terms of them. However, \mathcal{M}_{intr} is not, in general, an integral manifold of the distribution Ω determined

by the normal space $(T_x \mathcal{M}_{G/H})^{\perp}$, i.e. $(T_x \mathcal{M}_{G/H})^{\perp} \neq T_x \mathcal{M}_{intr}^{\dagger}$. Thus, in general $(Z_{\nu})_x$ are not in $(T_x \mathcal{M}_{G/H})^{\perp}$. Nevertheless, one may use the projector Λ in (3.11) to project $(Z_{\nu})_x$ into $(T_x \mathcal{M}_{G/H})^{\perp}$ and thereby obtain suitable vector fields in terms of which T_{intr} can be expressed. We shall use this construction in § 4.3 where we consider the special case $G = GL^+(3, \mathbb{R})$. In concluding this section we observe that the method presented here can easily be generalised to other spaces like \mathbb{R}^{kN} for arbitrary integer k (cf Eichinger 1977, Vanagas 1977) and other real and complex Riemannian manifolds.

4. $G = GL^+(3, \mathbb{R})$ The rotation-vibrational motion

In this section we apply the ideas of the previous section to $G = GL^+(3, \mathbb{R})$. We do this in some detail to emphasise the generality of the concepts used and to expose the pitfalls that may have gone unnoticed in some of the previous derivations. It has been shown previously (Gulshani and Rowe 1976, 1978, Gulshani 1977, 1978, 1981, Gulshani and Volkov 1981) that the general linear group $GL^+(3, \mathbb{R})$ is the kinematical group of collective monopole and quadrupole vibrations as well as irrotational and rigid rotational motions[‡]. These motions of an *N*-particle system are realised by identifying the collective and intrinsic submanifolds of \mathbb{R}^{3N} with the orbits and the orbit space of $GL^+(3, \mathbb{R})$ according to § 2. Now $GL^+(3, \mathbb{R})$ is isomorphic to the set of all (3×3) matrices with positive determinants and so acts naturally in \mathbb{R}^{3N} by matrix multiplication. Furthermore, we show in § 4.1, that for this action the isotropy subgroup H can be chosen the identity element in $GL^+(3, \mathbb{R})$ §. The orbit equation (2.11) then becomes

$$x^{ni} = g_{i\alpha}(y^{\omega})\bar{x}^{n\alpha}(\xi^{\sigma})$$
(4.1)

with $i, \alpha = 1, 2, 3; 1 \le \omega \le 9; 1 \le n \le N, 1 \le \sigma \le 3N - 9$ and $g \in GL^+(3, \mathbb{R})$. We note that the collective manifold \mathcal{M}_{GL} , i.e. the orbits of $GL^+(3, \mathbb{R})$, has dimension nine. According to § 2 the intrinsic manifold \mathcal{M}_{intr} in $\mathbb{R}^{3N} = \mathcal{M}_{GL} \times \mathcal{M}_{intr}$ is identified with the orbit space $\mathbb{R}^{3N}/GL^+(3, \mathbb{R})$ with $\bar{x} \in \mathcal{M}_{intr} = \mathbb{R}^{3N}/GL^+(3, \mathbb{R})$.

4.1. Collective and intrinsic manifolds

We now show that the isotropy subgroup H of $GL^+(3, \mathbb{R})$ can be chosen the identity element in $GL^+(3, \mathbb{R})$ and that the orbit space $\mathcal{M}_{intr} = \mathbb{R}^{3N}/GL^+(3, \mathbb{R})$ can be identified with a homogeneous space of the orthogonal group SO(N), called the Grassman

[‡] The more manageable two-dimensional collective motions described by $G = GL^+(2, \mathbb{R})$ can be similarly treated (see Bouten and Van Leuven (1977) for a different treatment).

§ Since the origin is a fixed point of this action, we exclude $\{0\} \in \mathbb{R}^{3N}$ as a first step in achieving an effective action.

⁺ In fact from the set $\{X_{\alpha}\}$ in (2.10) one can always construct a set of vector fields which span $(T_x \mathcal{M}_{G/H})^{\perp}$ (see appendix 1). But this set is, in general, not involutive. It then follows from the Frobenius' theorem (Auslander and MacKenzie 1963, p 147, Brickell and Clark 1970, p 197, Matsushima 1972, p 167, Boothby 1975, p 159) that Ω is non-integrable, i.e. there is no submanifold of \mathbb{R}^{3N} to which $(T_x \mathcal{M}_{G/H})^{\perp}$ is a tangent space.

^{||} Although the centre-of-mass motion is excluded from consideration in this paper, it can easily be incorporated in our journalism here. Its effect on our results here is obtained simply by letting $N \rightarrow N-1$ everywhere and regarding all coordinates and momenta to be defined relative to those of the centre of mass (cf Gulshani and Rowe 1976).

. ..

manifold of 3-planes[†]. An important step in this realisation is to use the vector space structure on \mathbb{R}^{3N} and to recognise (Surkov 1967, Dzyublik *et al* 1972, Morinigo 1972) that the 3N coordinates x^{ni} can be regarded as three vectors x^{i} in an abstract N-dimensional real vector space \mathbb{R}^{N} . The three linearly independent oriented vectors

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$$\begin{pmatrix} x^{1} \\ x^{2} \\ x^{3} \end{pmatrix} \equiv \begin{pmatrix} x^{11} & x^{21} & \dots & x^{N1} \\ x^{12} & x^{22} & \dots & x^{N2} \\ x^{13} & x^{23} & \dots & x^{N3} \end{pmatrix}$$
(4.2)

define what is known as an oriented 3-frame in \mathbb{R}^{N} . Each 3-frame determines a three-dimensional subspace of \mathbb{R}^{N} , called a 3-plane. Those 3-frames (4.2) which determine the same 3-plane, i.e. which are equivalent, are seen to be connected by $GL^{+}(3, \mathbb{R})$ as in (4.1). This is, of course, an equivalence relation on the set of all 3-frames. The set of all oriented 3-planes, i.e. the set of all three-dimensional subspaces of \mathbb{R}^{N} , can easily be shown, see below, to form a manifold, called the Grassman manifold of oriented 3-planes denoted by G(3, N) (see Auslander and MacKenzie 1963, p 176, Brickell and Clark 1970, pp 28, 92, 252, Matsushima 1972, p 241, Boothby 1975, pp 63, 167)‡. It therefore follows that the intrinsic manifold \mathcal{M}_{intr} of which \bar{x} in (4.1) is a point can be identified with the Grassman manifold of 3-planes G(3, N). With the interpretation of \mathcal{M}_{intr} as a manifold of oriented 3-planes we see that the isotropy subgroup H of $GL^{+}(3, \mathbb{R})$ in (4.1) is the identity element§. Therefore, the collective rotation-vibration submanifold \mathcal{M}_{GL} of \mathbb{R}^{3N} is identified with the 9-dimensional orbits of $GL^{+}(3, \mathbb{R})$ as in (4.1).

It is now simple to show that $\mathcal{M}_{intr} = G(3, N)$ is a manifold of dimension 3(N-3) diffeomorphic to a quotient manifold of the orthogonal group SO(N). Evidently G(3, N) is a homogeneous space of $GL^+(N, \mathbb{R})$ since $GL^+(N, \mathbb{R})$ acts transitively on G(3, N). Thus one can readily identify G(3, N) with a quotient space of $GL^+(N, \mathbb{R})$ (Matsushima 1972, p 241, Boothby 1975, p 167). Instead, however, it is more useful for practical purposes to use the inner-product structure on \mathbb{R}^N and identify $\mathcal{M}_{intr} = G(3, N)$ with a quotient space of SO(N). Because of the equivalence relation on G(3, N) given by the action of GL(3, $\mathbb{R})$ in (4.1), an arbitrary 3-plane, i.e. a point of G(3, N), is equivalent to some oriented orthonormal 3-plane. An orthonormal 3-plane defined by (cf. (4.2)) the $(3 \times N)$ matrix

$$\vec{x} = \begin{pmatrix} \vec{x}^{1} \\ \vec{x}^{2} \\ \vec{x}^{3} \end{pmatrix} = \begin{pmatrix} \vec{x}^{11} & \dots & \vec{x}^{N1} \\ \vec{x}^{12} & \dots & \vec{x}^{N2} \\ \vec{x}^{13} & \dots & \vec{x}^{N3} \end{pmatrix}$$
(4.3)

satisfies the scalar product

$$(\bar{x}^{\alpha}, \bar{x}^{\beta}) \equiv \sum_{n=1}^{N} \bar{x}^{n\alpha} \bar{x}^{n\beta} = \delta^{\alpha\beta} \qquad \alpha, \beta = 1, 2, 3.$$
(4.4)

[†] It ought to be mentioned that some interesting results on the properties of the intrinsic space have been obtained by Buck *et al* (1979) using the method of dyadics.

[‡] The properties of Grassman manifolds have been examined in detail in the mathematical literature (see Wolf 1963, 1967, Porteous 1969).

§ If one identifies \mathcal{M}_{intr} with the manifold of 3-frames, called the Stiefel manifold, then the isotropy subgroup of GL⁺(3, **R**) is SO(3) (see § 4.3 and appendix 2 for details).

Now SO(N) acts transitively on G(3, N), via matrix multiplication, taking one orthonormal 3-plane into another[†]. The isotropy subgroup H of SO(N) at the point

$$\omega = \begin{pmatrix} 1 & 0 & \cdot & \cdot & \dots & 0 \\ 0 & 1 & 0 & \cdot & \dots & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 \end{pmatrix} \equiv (I|0) \in \mathbf{G}(3, \mathbf{N}),$$

where I is the unit (3×3) matrix, is clearly given by

$$\mathbf{H} = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \qquad A \in \mathrm{SO}(3), \ B \in \mathrm{SO}(N-3)$$

because $\omega \cdot H = (A|0)$ is again an orthonormal 3-frame which lies in the 3-plane determined by ω . Since H is isomorphic to the direct product $SO(3) \times SO(N-3)$, it follows that $G(3, N) = \mathcal{M}_{intr}$ is diffeomorphic to the quotient manifold $SO(N) \setminus (SO(3) \times SO(N-3))$ of right cosets with dimension = dim $SO(N) - \dim SO(3) - \dim SO(N-3) = 3(N-3)$ (Clark and Brickell 1972, p 252, Matsushima 1972, p 241, Boothby 1975, p 358).

It then follows from the above arguments that the configuration space \mathbb{R}^{3N} decomposes into the product $\mathbb{R}^{3N} = \mathcal{M}_{GL} \times \mathcal{M}_{intr} = GL^+(3, \mathbb{R}) \times G(3, N)$. Equation (4.1) is then rewritten as

$$x^{ni} = g_{i\alpha}R_{\alpha n}, g \in \operatorname{GL}^+(3, \mathbb{R}), R \in \operatorname{SO}(N) \setminus (\operatorname{SO}(3) \times \operatorname{SO}(N-3))$$
(4.5)

with

$$R_{\alpha n}R_{\beta n} = \delta_{\alpha\beta} \qquad \qquad \alpha, \beta = 1, 2, 3. \tag{4.6}$$

From equations (4.6) and (4.5) we then have

$$Q_{ij} \equiv M x^{n_i} x^{n_j} = M g_{i\alpha} g_{j\alpha} \tag{4.7}$$

where Q is the mass quadrupole tensor of the N-particle system. Equation (4.7) defines in \mathbb{R}^{3N} only six of the nine matrix elements of $g \in \mathrm{GL}^+(3, \mathbb{R})$. The remaining three elements can be defined in \mathbb{R}^{3N} almost arbitrarily (see § 4.3 for a forbidden choice).

4.2. Collective momenta and kinetic energy

The direct-sum decomposition

$$T_{\mathfrak{x}}\mathbb{R}^{3N} = T_{\mathfrak{x}}\mathcal{M}_{\mathrm{GL}} \oplus (T_{\mathfrak{x}}\mathcal{M}_{\mathrm{GL}})^{\perp}$$

$$(4.8)$$

for the particle momenta p_{ni} and the corresponding decomposition of the total kinetic energy into collective and intrinsic parts are now easily obtained from the procedure given in §4.3. We first need to compute the infinitesimal operators t of $GL^+(3, \mathbb{R})$ on \mathcal{M}_{GL} according to the prescription (2.10). A natural coordinate chart on $GL^+(3, \mathbb{R})$ is given by the elements g_{ij} of the matrix $g \in GL^+(3, \mathbb{R})$. Using the rule (2.10) and

 $[\]dagger$ Note that this is a right action arising from our choice of the 3-frames to be represented by three rows rather than three columns (cf (4.3)).

equation (4.1) (or 4.5)), we have

$$t_{ij} = \psi_{\bar{x}}^* \left(\frac{\partial}{\partial g_{ji}}\right)_e = \left[\frac{\partial}{\partial g_{ji}} \left(x^{nk} \circ \psi_{\bar{x}}(g)\right)\right]_e \frac{\partial}{\partial x^{nk}}$$
$$= \left[\frac{\partial}{\partial g_{ji}} \left(g_{k\alpha} \bar{x}^{n\alpha}\right)\right]_e \frac{\partial}{\partial x^{nk}}$$
$$= x^{ni} \frac{\partial}{\partial x^{nj}}.$$
(4.9)

The set $\{t_{ij}\}$ spans at each $x \in \mathbb{R}^{3N}$ the nine-dimensional subspace $T_x \mathcal{M}_{GL}$ of $T_x \mathbb{R}^{3N}$. Comparing (4.9) with (2.10), we find that the components X_{ij}^{nk} of t_{ij} with respect to the basis $\{\partial/\partial x^{nk}\}$ for $T_x \mathbb{R}^{3N}$ are given by

$$X_{ij}^{nk} = x^{ni}\delta_{jk}.\tag{4.10}$$

The induced metric h on the $\operatorname{GL}^+(3,\mathbb{R})$ orbit $\mathcal{M}_{\operatorname{GL}}$ is then computed from (3.3) and (4.10) to be

$$h_{ij,lk} \equiv g(t_{ij}, t_{lk}) = M^{-1} Q_{il} \delta_{jk}$$
(4.11)

with the inverse

$$h^{ij,lk} = MQ_{ij}^{-1}\delta_{jk} \tag{4.12}$$

where Q^{-1} is the inverse of the mass quadrupole tensor Q defined in (4.7). Q^{-1} can easily be expanded in terms of minors to obtain

$$Q_{ij}^{-1} = \frac{1}{2 \det Q} \left[\delta_{ij} (\operatorname{Tr} Q)^2 - \delta_{ij} \operatorname{Tr} Q^2 - 2(\operatorname{Tr} Q) Q_{ij} + 2Q_{ij}^2 \right]$$
(4.13)

whence

det
$$Q = \frac{1}{6} [(\text{Tr } Q)^3 - 3(\text{Tr } Q)(\text{Tr } Q^2) + 2 \text{ Tr } Q^3].$$

From the definition (3.4) and equations (4.10) and (3.12) the projection operator

 $\overline{\Gamma} = T_{x} \mathbb{R}^{3N} \twoheadrightarrow T_{x} \mathcal{M}_{\mathrm{GL}}$

is then given by the $(3N \times 3N)$ matrix

$$\bar{\Gamma}_{ni,mj} \equiv X_{lk}^{ni} h^{lk,lk} X_{lk}^{mj} \equiv \delta_{ij} \Gamma_{nm}$$
(4.14*a*)

where

$$\Gamma_{nm} \equiv M x^{nl} Q_{lk}^{-1} x^{mk}. \tag{4.14b}$$

From (4.7) and (3.14) we can easily ascertain that $\overline{\Gamma}$ has the requisite properties: it is a symmetric, idempotent matrix and rank $\overline{\Gamma} = \operatorname{Tr} \overline{\Gamma} = 9 = \dim \operatorname{GL}^+(3, \mathbb{R}) = \dim(T_x \mathcal{M}_{GL})$. In (4.14*a*) we observe the curious splitting of $\overline{\Gamma}$ into the product of the Kronecker delta function and the $(N \times N)$ matrix Γ . From (4.14*b*) it can easily be shown that Γ is symmetric and idempotent and rank $\Gamma = \operatorname{Tr} \Gamma = 3$. What geometric property underlies the splitting in (4.14*a*) is not clear yet[†].

[†] As a consequence of this splitting, however, one can easily show that the set of all matrices $\overline{\Gamma}$ in (4.14*a*) is diffeomorphic to the Grassman manifold SO(N)(SO(3)×SO(N-3)).

The decomposition (4.8) of the particle momentum space is now obtained simply by substituting (4.14*a*) into (3.10). One finds^{\dagger}

$$p_{ni} \equiv -i\hbar \frac{\partial}{\partial x^{ni}} = \Gamma_{nm} p_{mi} + \Lambda_{nm} p_{mi} \equiv p_{ni}^{\text{coll}} + p_{ni}^{\text{intr}}$$
(4.15*a*)

where

$$p_{ni}^{\text{coll}} = \Gamma_{nm} p_{mi} = -i\hbar M x^{nl} Q_{lk}^{-1} t_{ki}$$
(4.15b)

and

$$\Lambda_{nm} \equiv \delta_{nm} - \Gamma_{nm}. \tag{4.16}$$

The corresponding decomposition of the total kinetic energy into collective and intrinsic parts is obtained by substituting (4.14a) into (3.13). One finds

$$T = \frac{1}{2M} \sum_{ni} p_{ni}^2 = \frac{1}{2M} p_{ni} \Gamma_{nm} p_{mi} + \frac{1}{2M} p_{ni} \Lambda_{nm} p_{mi}$$
$$= T_{\text{coll}} + T_{\text{intr}}$$
(4.17*a*)

where

$$T_{\rm intr} = \frac{1}{2M} p_{ni} \Gamma_{nm} p_{mi} = \frac{1}{2M} \sum_{ni} (p_{ni}^{\rm intr})^2$$
(4.17b)

and

$$T_{\rm coll} = \frac{1}{2M} p_{ni} \Gamma_{nm} p_{ni} = -\frac{1}{2} \hbar^2 [t_{ki} Q_{kl}^{-1} t_{li} + N Q_{ik}^{-1} t_{ki}].$$
(4.17c)

It is important to note the definitions of T_{coll} and T_{intr} in (4.17) and their relations to p_{ni}^{coll} and p_{ni}^{intr} in (4.15). $T_{\text{intr}} = (1/2M) \sum_{ni} (p_{ni}^{\text{intr}})^2$ because the term $p_{ni}^{\text{coll}} p_{ni}^{\text{intr}} = 0$ but $T_{\text{coll}} \neq (1/2M) \sum_{ni} (p_{ni}^{\text{coll}})^2$ because $p_{ni}^{\text{intr}} p_{ni}^{\text{coll}} \neq 0$, the orthogonality condition $g(p_{ni}^{\text{coll}}, p_{mj}^{\text{intr}}) = 0$ notwithstanding.

The physical content of the expressions (4.15b) and (4.17c) for p_{ni}^{coll} and T_{coll} is revealed by a transformation to the mass quadrupole principal axes. These three axes, which will be indicated by suffixes A, B and C, are given by the diagonalisation of the symmetric second-rank tensor Q in (4.7)

$$r_{Ai}r_{Bj}Q_{ij} \equiv \delta_{AB}I_A \qquad A, B = 1, 2, 3 \tag{4.18}$$

where $r \in SO(3)/D_2$ and D_2 , the dihedral group (Hamermesh 1962), is the isotropy discrete subgroup of SO(3) consisting of the identity element and rotations through angle π about each of the three axes leaving the diagonal matrix with elements I_A invariant. In (4.18) I_A are the three mass quadrupole principal moments defined by

$$\delta_{AB}I_{A} = M \sum_{n=1}^{N} x^{nA} x^{nB} \qquad x^{nA} \equiv r_{Ai} x^{ni}.$$
(4.19)

The transformation of T_{coll} in (4.17c) to the quadrupole principal axes is clearly equivalent to choosing on the $GL^+(3, \mathbb{R})$ manifold the coordinate system given by the decomposition (Gantmacher 1960)

$$g_{i\alpha} \equiv r_{Ai} S_A \bar{r}_{A\alpha} \qquad S_A = (I_A/M)^{1/2} \qquad (4.20)$$

 \ddagger Note that the centre-of-mass projector is $N^{-1} \delta_{nm} \delta_{ij}$.

with $g \in GL^+(3, \mathbb{R})$ and $r, \bar{r} \in SO(3)/D_2$, and repeating the above analysis starting from (4.9). We have chosen S_A in (4.20) so that equations (4.7) and (4.18) are satisfied. Moreover, for uniqueness of the decomposition (4.20) we choose the ordering $I_3 \ge I_1 \ge I_2$. With two sets of Euler angles $\{\theta_A\}$ and $\{\phi_A\}$ and the three parameters S_A as coordinates the new set of nine infinitesimal operators of $GL^+(3, \mathbb{R})$ are computed from (2.10), (4.1), (4.20) to be the orbital angular momentum

$$L_{A} = \left(\frac{\partial r_{Bi}}{\partial \theta_{A}} S_{B} \bar{r}_{B\alpha} \bar{x}^{n\alpha}\right)_{e} \frac{\partial}{\partial x^{ni}} = \varepsilon_{ABC} t_{BC}$$
(4.21*a*)

the dilation momenta

$$t_{A} = \left(r_{Bi} \frac{\partial S_{B}}{\partial S_{A}} \bar{r}_{B\alpha} \bar{x}^{n\alpha} \right)_{e} \frac{\partial}{\partial x^{ni}} = t_{AA}$$
(4.21*b*)

the shear angular momentum

$$\mathscr{L}_{A} = \left(r_{Bi} S_{B} \frac{\partial \tilde{r}_{B\alpha}}{\partial \phi_{A}} \bar{x}^{n\alpha} \right)_{e} \frac{\partial}{\partial x^{ni}} = \varepsilon_{ABC} \left(\frac{I_{C}}{I_{B}} \right)^{1/2} t_{BC}$$
(4.21c)

where ε is the permutation symbol and t_{AB} are the principal-axis components of t_{ij} in (4.9) defined by

$$t_{AB} \equiv r_{Ai} r_{Bi} t_{ij} \equiv x^{nA} \, \partial/\partial x^{nB} \tag{4.22}$$

with x^{nA} given in (3.18) and $\partial/\partial x^{nA} \equiv r_{Ai} \partial/\partial x^{ni}$. The operators in (4.21) are related to their respective space-fixed components as follows

$$L_i = r_{Ai}L_A \qquad \qquad \mathcal{L}_i = r_{Ai}\mathcal{L}_A \qquad \qquad t_A \equiv t_{AA} = r_{Ai}r_{Aj}t_{ij}. \tag{4.23}$$

Equations (4.21) are seen to be related in a linear manner to the two sets of basis vectors $\{L_A, t_A, \mathcal{L}_A\}$ and $\{t_{AB}\}$ for $T_x \mathcal{M}_{GL}$.

From the basis set of operators in (4.21) one can now construct a projection matrix operator similar to $\overline{\Gamma}$ in (4.14*a*) and proceed to obtain p_{ni}^{coll} and T_{coll} in (4.15*b*) and (4.17*c*) in terms of the operators (4.21). This calculation is not reproduced here because the result is more easily obtained by expressing p_{ni}^{coll} and T_{coll} first in terms of $\{t_{AB}\}$ and then in terms of the set $\{L_A, t_A, \mathcal{L}_A\}$. The result for T_{coll} is[†]

$$T_{\rm coll} = T_{\rm vib} + T_{\rm rot} \tag{4.24a}$$

where

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

$$T_{\rm rot} = -\frac{\hbar^2}{2} \sum_{A < B}^3 \left[\frac{I_A + I_B}{(I_A - I_B)^2} \left(L_{AB}^2 + \mathcal{L}_{AB}^2 \right) - \frac{4\sqrt{I_A I_B}}{(I_A - I_B)^2} L_{AB} \mathcal{L}_{AB} \right] \quad (4.24c)$$

and

$$L_{AB} \equiv L_C$$
 $\mathscr{L}_{AB} \equiv \mathscr{L}_C$ A, B, C in cyclic order.

In (4.24b) we have used the identity $t_A \equiv t_{AA} = 2I_A \partial/\partial I_A$ obtained from the chain rule $\partial/\partial I_A = (\partial x^{ni}/\partial I_A)(\partial/\partial x^{ni})$ and equations (4.20) and (4.5). The collective kinetic energy

 p_{ni}^{coll} can be written as a sum of two terms, one describing irrotational and the other rigid flow. The detail of this has been given elsewhere (Gulshani and Rowe 1976, 1978, Gulshani 1978, Gulshani and Volkov 1981).

(4.24) has been derived previously by the present authors and others who used coordinate transformations and different decompositions of \mathbb{R}^{3N} and $T_x \mathbb{R}^{3N}$ from the one given here (Zickendraht 1971, Dzyublik *et al* 1972, Gulshani and Rowe 1976, Ovcharenko 1976, Vanagas 1977, Gulshani 1978, 1981, Weaver *et al* 1976, Buck *et al* 1979). As may be observed T_{coll} in (4.24) represents physically the kinetic energy of vibrational and rotational motions. It is also reducible to that of Bohr's nuclear collective model (Bohr 1952) as shown previously (Zickendraht 1971, Gulshani and Rowe 1976, Gulshani 1978, Gulshani and Volkov 1981). With the help of (4.13) the relation of T_{coll} in (4.24) and (4.17c) to the spectrum-generating algebras $cm(3) \sim \mathbb{R}^6 + gl(3, \mathbb{R}) \equiv \{Q, t\}, gl(3, \mathbb{R}) \equiv \{t\}$ and $\mathbb{R}^6 + so(3) \equiv \{Q, L\}$ also becomes apparent (Gulshani and Rowe 1976).

The Hilbert space for the $GL^+(3, \mathbb{R})$ collective model (4.17c) and (4.24) is spanned by a set of square-integrable functions defined on $GL^+(3, \mathbb{R})$. From (4.24) and (4.20) this set is seen to be given by the functions $\mathscr{I}_{K\mathcal{R}\lambda}^{L\mathscr{G}}(I_A) \mathscr{D}_{MK}^L(r) \mathscr{D}_{\mathscr{R}\mathcal{R}}^{\mathscr{G}}(r)$ where the \mathscr{D} are the Wigner rotation matrices and \mathscr{I} some square-integrable functions of I_A labelled by indices λ . Because of the invariance with respect to the D₂ group in (4.20) and (4.24), the symmetrised basis functions become (cf Bohr 1952, Kumar and Baranger 1967, Eisenberg and Greiner 1970a, p 147, Bohr and Mottelson 1975, p 178)

$$\Phi_{\mathcal{M}\mathcal{M}\mathcal{K}\mathcal{K}\lambda}^{\mathcal{L}\mathcal{L}}(g) \equiv \mathscr{J}_{\mathcal{K}\mathcal{K}\lambda}^{\mathcal{L}}(I_A) [\mathscr{D}_{\mathcal{M}\mathcal{K}}^{\mathcal{L}}(r) \mathscr{D}_{\mathcal{M}\mathcal{K}}^{\mathcal{L}}(\bar{r}) + (-1)^{L+K+\mathcal{L}+\mathcal{K}} \mathscr{D}_{\mathcal{M}-K}^{\mathcal{L}}(r) \mathscr{D}_{\mathcal{M}-\mathcal{K}}^{\mathcal{L}}(\bar{r})]$$
(4.25)

with r, $\bar{r} \in SO(3)/D_2$ and $g \in GL^+(3, \mathbb{R})$. These functions span the irreducible representation of the group CM(3) obtained by Weaver *et al* (1976). The functions \neq in (4.25), the collective energy spectrum, the electric quadrupole transition rates, etc are then calculated from the eigenvalue problem for the collective Hamiltonian H_{coll} = $T_{\rm coll} + V_{\rm coll}$. The collective potential $V_{\rm coll}$ can be chosen a polynomial in the three well-known $\mathbb{R}^6 \otimes SO(3)$ invariants $I^{(1)} \equiv \text{Tr } Q = I_1 + I_2 + I_3$, $I^{(2)} \equiv \frac{1}{2} \text{Tr } Q^2 = \frac{1}{2}(I_1^2 + I_2^2 + I_3^2)$ and $I^{(3)} \equiv \frac{1}{3} \text{Tr } Q^3 = \frac{1}{3}(I_1^3 + I_2^3 + I_3^3)$ (Kumar and Baranger 1967, Noack 1968, Eisenberg and Greiner 1970a, p 45, Ui 1970, Spencer 1971, Chacón and Moshinsky 1977). However, because of the complexity of the differential operators (4.24), calculations for only simple cases have so far been carried out (Zickendraht 1971, Filippov 1974, Filippov and Maksimenko 1975, Gulshani and Volkov 1981). $H_{\rm coll}$ may also be diagonalised in some approximation using (4.17c) and the expansion (4.13) for Q^{-1} (cf Gulshani and Volkov 1981) within an irreducible representation of the symplectic group Sp(6, \mathbb{R}) (Asherova *et al* 1976) based on Elliot's SU(3) harmonic oscillator basis (Elliot 1958, Harvey 1968). This latter recourse has the desirable feature of being microscopic, i.e. relates the collective eigenstates to those of the independent particles. Perhaps a more appropriate basis for the diagonalisation of H_{coll} is provided by an irreducible representation of the direct-product group $SU(6) \times SO(3)$. Here the group SU(6) describes the boson part of H_{coll} obtained by expressing T_{coll} in (4.17c) in terms of the momentum canonically conjugate to Q given by one of the authors (Gulshani 1978). This description makes a direct contact with and may in fact generalise the highly successful nuclear Interacting Boson Model (Arima and Iachello 1975, 1976, 1978, Iachello 1979) as will be shown in a subsequent paper.

4.3. Intrinsic momenta and kinetic energy

For a unified and consistent formulation of the problem of the intrinsic and the CM(3) collective motion given in §§ 4.1 and 4.2 it is now necessary to obtain a set of (3N-9) basis vectors for the normal space $(T_x \mathcal{M}_{GL})^{\perp}$ in (4.8) in terms of a set of vectors $\{J\}$ on the

Grassman manifold of 3-planes $G(3, N) = \mathcal{M}_{intr} in (4.5)$. The aim is then to express p_{ni}^{intr} in (4.15a) and $T_{intr} in (4.17b)$ in terms of (3N-9) intrinsic vector fields on \mathcal{M}_{intr} . With some caution to avoid pitfalls this can be accomplished rather simply as we now show.

From the rule (2.10) and the diffeomorphism between G(3, N) and SO(N)\(SO(3) × SO(N-3)) given in § 4.1 (cf (4.5)) one readily finds that the vector fields $\{J\}$ on \mathcal{M}_{intr} are given by

$$J_{nm} \equiv x^{ni} \frac{\partial}{\partial x^{mi}} - x^{mi} \frac{\partial}{\partial x^{ni}}.$$
(4.26)

It ought to be emphasised that J_{nm} are not defined on the SO(N) manifold. But they are defined on SO(N)\SO(N-3). This latter circumstance arises from the fact that SO(N) acts transitively on the set of all oriented orthonormal 3-frames S(3, N) in (4.2) with the isotropy subgroup SO(N-3). Indeed, from an analysis similar to that given for G(3, N) in § (4.1) one can show that S(3, N) is a manifold of dimension (3N-6) diffeomorphic to the quotient manifold SO(N)\SO(N-3) of right cosets. S(3, N) is known as the Stiefel manifold of 3-frames (Auslander and MacKenzie 1963, p 175, Brickell and Clark 1970, pp 92, 253, Warner 1971, p 129)[†]. Furthermore, we see that G(3, N) arises from defining the following equivalence relation on S(3, N): $x \sim y$ if $y = x \cdot r$ for $r \in SO(3)$ and $x, y \in S(3, N)$ (see also appendix 2).

Now the vector fields J_{nm} in (4.26) on \mathcal{M}_{intr} are not orthogonal to the vector fields t_{ij} in (4.9) on \mathcal{M}_{GL} because the inner product $g(t_{ij}, J_{nm}) = x^{mi}x^{nj} - x^{ni}x^{mj}$ does not vanish for $i \neq j$. Therefore, $\mathcal{M}_{intr} = \mathbf{G}(3, N)$ is not an integral manifold of the distribution determined by $(T_x \mathcal{M}_{GL})^{\perp}$, i.e. $(T_x \mathcal{M}_{GL})^{\perp} \neq T_x \mathcal{M}_{intr}$. If one were to require that $(T_x \mathcal{M}_{GL})^{\perp} = T_x \mathbf{G}(3, N)$ as was done previously (Gulshani and Rowe 1976), one would arrive at the conclusion that every coordinate system on $\mathbf{G}(3, N)$ is non-integrable on \mathbb{R}^{3N} as is shown in appendix 3. However, we can use the $gl(3, \mathbb{R})$ projector Λ in (4.16) to project J_{nm} onto the normal space $(T_x \mathcal{M}_{GL})^{\perp}$. Thus the vector fields

$$\bar{J}_{nm} \equiv \Lambda_{n\bar{m}} J_{m\bar{m}} \tag{4.27}$$

are in $(T_x \mathcal{M}_{GL})^{\perp}$ since the scalar product $g(t_{ij}, \overline{J}_{nm}) = \Lambda_{nm} x^{mi} x^{mj} = 0$ for all *i*, *j*, *n* and *m* by virtue of the relations

$$\Gamma_{nm} x^{mj} = x^{nj} \qquad \Lambda_{nm} x^{mj} = 0 \qquad \text{for all } n \text{ and } j. \tag{4.28}$$

The result in (4.28) follows readily from the definitions (4.7), (4.14b) and (4.16). The operators (4.27) are then vector fields along but not on (tangent to) $\mathcal{M}_{intr} = G(3, N)$.

By means of a simple algebraic manipulation one can now express p_{ni}^{intr} in (4.15*a*) and T_{intr} in (4.17*b*) in terms of the intrinsic vector fields (4.27). Substituting the identity (cf (4.7))

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

into p_{ni}^{intr} and using (4.28) one can easily show that

$$p_{ni}^{\text{intr}} \equiv \Lambda_{nm} p_{mi} = -i\hbar \sqrt{M} Q_{ik}^{-1/2} \tilde{J}_{kn}$$
(4.29)

where

$$\bar{J}_{kn} \equiv \bar{R}_{km}\bar{J}_{nm} \tag{4.30}$$

[†] Evidently S(k, N) for any integer $k \le N$ is a generalisation of the unit sphere. In particular the unit N-sphere in \mathbb{R}^N is $S^{N-1} = S(1, N)$ (cf Vilenkin 1968) and the unit 2-sphere in \mathbb{R}^3 is $S^2 = S(1, 3)$. A natural coordinate chart on S(3, N) is then given by generalised spherical coordinates (cf Vilenkin 1968, Dzyublik *et al* 1972, Ovcharenko 1976).

and

$$\bar{R}_{in} \equiv \sqrt{M}Q_{ik}^{-1/2} x^{nk} \tag{4.31}$$

where \overline{J}_{nm} is as in (4.27). $Q^{-1/2}$ in (4.29) and (4.31) is the inverse of $Q^{1/2}$ defined in terms of the principal moments I_A in (4.18) by

$$Q_{ij}^{1/2} \equiv r_{Ai} r_{Aj} (I_A)^{1/2} \qquad Q_{ij}^{-1/2} \equiv r_{Ai} r_{Aj} (I_A)^{-1/2}.$$
(4.32)

One now uses the commutation relations

$$[J_{nm}, x^{\bar{n}i}] = (\delta_{m\bar{n}} x^{ni} - \delta_{n\bar{n}} x^{mi})$$
(4.33)

and, hence,

$$[J_{nm}, Q_{ij}] = 0$$
 for all *n*, *m*, *i* and *j* (4.34)

to obtain

$$T_{\rm intr} = \frac{1}{2M} \sum_{ni} (p_{ni}^{\rm intr})^2 = -\frac{1}{2} \hbar^2 \tilde{J}_{in} Q_{ij}^{-1} \tilde{J}_{jn}, \qquad (4.35)$$

Transforming (4.35) to the quadrupole principal axes in (4.18) and using the commutators (cf (4.34) and (4.18))

$$[J_{nm}, I_A] = [J_{nm}, r_{Ai}] = 0 (4.36)$$

one obtains

$$T_{\rm intr} = -\frac{1}{2}\hbar^2 \sum_{n,A} \frac{1}{I_A} \bar{J}_{An}^2$$
(4.37)

where

$$\bar{J}_{An} \equiv r_{Ai}\bar{J}_{in} \equiv \Lambda_{nm}J_{Am} \tag{4.38}$$

$$J_{AM} \equiv \bar{R}_{An} J_{nm} \tag{4.39}$$

and

$$\bar{R}_{Am} \equiv r_{Ai}\bar{R}_{im} \equiv (M/I_A)^{1/2} x^{nA}.$$
(4.40)

Equation (4.40) follows directly from (4.32), (4.31) and (4.19).

Geometrically \bar{R}_{An} in (4.40) is a point of S(3, N), the Stiefel manifold of orthonormal 3-frames (cf (4.43) below). From the diffeomorphism $S(3, N) = SO(N) \setminus SO(N-3)$ established above it follows that \bar{R}_{Am} are three rows of an $(N \times N)$ orthogonal matrix $\bar{R} \in SO(N) \setminus SO(N-3)$. Furthermore, \bar{R}_{Am} effects the transformation from the axes in \mathbb{R}^N labelled by (n, m, ...) to the three principal axes (A, B, C) of the projection matrix Γ in (4.14b). This is seen from the definition of Γ , which can be rewritten in the form

$$\Gamma_{nm} = \bar{R}_{in}\bar{R}_{im} = \bar{R}_{An}\bar{R}_{Am} \tag{4.41}$$

and from the fact that Γ can be brought, up to an ordering of the eigenvalues, to the diagonal form

$$\Gamma^{0} \equiv \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} = \bar{R}^{T} \Gamma \bar{R}$$
(4.42)

for some $\bar{R} \in SO(N) \setminus SO(N-3)$ with SO(N-3) being the isotropy subgroup of SO(N)

at Γ^{0} [†]. As expected one can easily verify the following properties (cf (4.19), (4.33), (4.34), (4.36) and (4.40)):

$$\bar{R}_{An}\bar{R}_{Bn} = \delta_{AB} \tag{4.43}$$

$$\Gamma_{nm}\bar{R}_{Am} = \bar{R}_{An} \tag{4.44}$$

$$[J_{nm}, \bar{R}_{A\bar{n}}] = \delta_{m\bar{n}}\bar{R} - \delta_{n\bar{n}}\bar{R}_{Am}.$$

$$(4.45)$$

Now using equations (4.16) and (4.43)–(4.45) and the properties

$$\Gamma_{nm}\Lambda_{m\bar{n}} = \Lambda_{nm}\bar{R}_{Am} \equiv 0 \tag{4.46}$$

(cf (4.28)), we can simplify the expression (4.37) for T_{intr} and obtain

$$T_{\rm intr} = -\frac{1}{2}\hbar^2 \sum_{A} \frac{1}{I_A} \left(\sum_{n} J_{An}^2 - \sum_{B} J_{AB}^2 \right)$$
(4.47)

where

$$J_{AB} \equiv \bar{R}_{An} \bar{R}_{Bm} J_{nm}. \tag{4.48}$$

The expression (4.47) for T_{intr} is, however, not in a convenient form because the operators J_{An} are components of J_{nm} along two different sets of axes: the axes (n, m) in \mathbb{R}^N and the three axes (A, B, C) of the N principal axes of Γ . Clearly one can remedy this situation by using the remaining (N-3) rows $\bar{R}_{\nu n}(4 \le \nu \le N)$ of the matrix $\bar{R} \in SO(N) \setminus SO(N-3)$ of which \bar{R}_{An} in (4.40) is the first three rows. But one must now exercise some caution. The rows $\bar{R}_{\nu n}$ have the obvious definition (cf (4.46), (4.43), (4.41) and (4.16))[‡]

$$\bar{R}_{An}\bar{R}_{\nu n}=0 \qquad \bar{R}_{\mu n}\bar{R}_{\nu n}=\delta_{\mu \nu} \qquad 4 \le \mu, \, \nu \le N \tag{4.49}$$

$$\Lambda_{nm} = \delta_{nm} - \bar{R}_{An} \bar{R}_{Am} = \bar{R}_{\nu n} \bar{R}_{\nu m}. \tag{4.50}$$

Equations (4.49) and (4.50) do not determine $\bar{R}_{\nu n}$ uniquely. Thus, unlike \bar{R}_{An} in (4.40), $\bar{R}_{\nu n}$ are not uniquely defined functions of the coordinates x^{ni} on \mathbb{R}^{3N} . However, the real difficulty in using $\bar{R}_{\nu n}$ in (4.47) is that, for any arbitrarily constructed $\bar{R}_{\nu n}$ satisfying (4.49) and (4.50), $\bar{R}_{\nu n}$ do not have simple transformation properties under the action of J_{nm} in (4.26). For example, it has been shown (Gulshani 1981, appendix 1) that

$$[J_{nm}, \bar{R}_{\nu\bar{n}}] \neq \delta_{m\bar{n}} \bar{R}_{\nu n} - \delta_{n\bar{n}} \bar{R}_{\nu m}$$

$$\tag{4.51}$$

in contrast to the transformation properties of \bar{R}_{An} in (4.45). Related to the inequality (4.51) is the nullity, $J_{\mu\nu} \equiv \bar{R}_{\mu n} \bar{R}_{\nu m} J_{nm} \equiv 0$, of the components of J_{nm} along (N-3) of the N principal axes of Γ (cf (4.26), (4.28) and (4.50)). This is simply a generalisation of the situation in \mathbb{R}^3 where the component of the angular momentum along the radius vector vanishes.

Recalling the distinction between the angular momentum of a single particle and that of a rigid body in \mathbb{R}^3 , we now introduce in juxtaposition with J_{nm} the infinitesimal operators K_{nm} of SO(N). One can now show (Ovcharenko 1976, and cf SO(3) cases) that the operators J_{nm} and K_{nm} become identical when acting on functions Ψ defined on

[†] The set of all matrices $\{\Gamma\}$ is seen to be diffeomorphic to $SO(N)\setminus SO(N-3)$.

 $[\]ddagger \bar{R}_{\nu n}$ are seen to be the (N-3) eigenvectors of Γ and Λ with eigenvalues zero and unity respectively.

The former momentum is defined on SO(3)/SO(2) whereas the latter is defined on SO(3) (see Gulshani 1979 and references therein).

 $SO(N) \setminus SO(N-3)$, i.e.

$$J_{nm}\Psi(\bar{R}) = K_{nm}\Psi(\bar{R}) \qquad \bar{R} \in \mathrm{SO}(N) \backslash \mathrm{SO}(N-3). \tag{4.52}$$

It can also be shown that, for any $\overline{R}_{\nu n} \in SO(N)^{\dagger}$,

$$[K_{nm}, \bar{R}_{\nu\bar{n}}] = \delta_{m\bar{n}}\bar{R}_{\nu n} - \delta_{n\bar{n}}\bar{R}_{\nu m}$$
(4.53)

(cf (4.51)). From (4.52) and (4.45) we also have

$$[K_{nm}, \bar{R}_{A\bar{n}}] = \delta_{m\bar{n}}\bar{R}_{A\bar{n}} - \delta_{n\bar{n}}\bar{R}_{m}.$$
(4.54)

We can now restrict the action of the operator T_{intr} in (4.47) to functions defined on SO(N) SO(N-3) and use equations (4.52) and (4.53) to simplify T_{intr} . Using the suffix σ to range over both suffixes A and ν , one then obtains

$$\sum_{n=1}^{N} J_{An}^{2} \Psi(\bar{R}) = \sum_{n=1}^{N} K_{AN}^{2} \Psi(\bar{R}) = \sum_{n,\sigma=1}^{N} \bar{R}_{\sigma n} K_{A\sigma} \bar{R}_{\bar{\sigma} n} K_{An} \Psi(\bar{R})$$
$$= \sum_{\sigma=1}^{N} K_{A\sigma}^{2} \Psi(\bar{R}) = \left(\sum_{\nu=1}^{N-3} K_{A\nu}^{2} + \sum_{B=1}^{3} K_{AB}^{2}\right) \Psi(\bar{R})$$
(4.55)

where $K_{A\nu}$ and K_{AB} are Γ principal-axis components of K_{nm} defined by

$$K_{A\nu} \equiv \bar{R}_{An} \bar{R}_{\nu m} K_{nm} \qquad K_{AB} \equiv \bar{R}_{An} \bar{R}_{Bm} K_{nm}. \tag{4.56}$$

To obtain the second line in (4.55) we have used (4.53). Substituting (4.55) into (4.47), one then readily obtains

$$T_{\rm intr}\Psi(\bar{R}) = -\frac{1}{2}h^2 \sum_{\nu=1}^{N-3} \sum_{A=1}^{3} \frac{1}{I_A} K_{A\nu}^2 \Psi(\bar{R}) \qquad \bar{R} \in \mathrm{SO}(N) \backslash \mathrm{SO}(N-3).$$
(4.57)

It is observed that T_{intr} in (4.57) is equally well defined on the (3N-9)-dimensional Grassman manifold SO(N)\(SO(3)×SO(N-3))). Furthermore, it is seen that only (3N-9) intrinsic vector fields $K_{A\nu}$ appear in (4.57) as desired[‡]. Using (4.19) and the definition of \bar{R}_{An} in (4.40), one can also express the GL⁺(3, R) infinitesimal operators \mathscr{L}_A in (4.21c) in terms of J_{nm} in (4.26). One obtains

$$\mathscr{L}_{C} = \bar{R}_{An} \bar{R}_{Bm} J_{nm} \qquad A, B, C \text{ in cyclic order.}$$
(4.58)

This relation can be understood in terms of the geometrical connection between the Grassman and the Stiefel manifolds mentioned before (see also appendix 2).

Combining (4.17a), (4.24), and (4.57) and (4.58), we finally obtain, for the total kinetic energy, the expression

$$T\Psi(\bar{R}) = -\frac{1}{2}\hbar^{2} \left\{ \sum_{\nu=1}^{N-3} \sum_{A=1}^{3} \frac{1}{I_{A}} K_{A\nu}^{2} + 4 \sum_{A=1}^{3} I_{A} \left[\frac{\partial^{2}}{\partial I_{A}^{2}} + \left(\frac{N-2}{2I_{A}} + \sum_{B\neq A}^{3} \frac{1}{I_{A} - I_{B}} \right) \frac{\partial}{\partial I_{A}} \right] + \sum_{A < B}^{3} \left[\frac{I_{A} + I_{B}}{(I_{A} - I_{B})^{2}} (L_{AB}^{2} + K_{AB}^{2}) - \frac{4\sqrt{I_{A}I_{B}}}{(I_{A} - I_{B})^{2}} L_{AB}K_{AB} \right] \right\} \Psi(\bar{R})$$

$$(4.59)$$

[†] Because $\bar{R}_{\nu n}$ in (4.49) and (4.50) is not uniquely defined, we may choose to define it either on SO(N) or SO(N)\SO(N-3). But to satisfy (4.53) $\bar{R}_{\nu n}$ must be defined on SO(N) (cf (4.52) and (4.51)).

[‡] It is seen to be a consequence of (4.51) that the operators $K_{A\nu}^2$ in (4.57) cannot be replaced by $J_{A\nu}^2$, where $J_{A\nu} = \bar{R}_{An}\bar{R}_{\nu m}J_{nm}$, in spite of the equality in (4.52) as was pointed out previously (Gulshani 1981).

where $\bar{R} \in SO(N) \setminus SO(N-3)$. Expression (4.59) has been given before (Gulshani 1981) and is identical to[†] that derived by Dzyublik *et al* (1972), Filippov (1974), Ovcharenko (1976) and Vanagas (1977) who used the chain-rule method and a different decomposition of \mathbb{R}^{3N} and $T_x \mathbb{R}^{3N}$ (see appendix 2). T in (4.59) is also similar to that given by Buck *et al* (1979) (see appendix 3). One of the merits of the expression (4.59) is the simple features of T_{intr} made possible by the introduction of the mathematically tractable SO(N) and its quotient manifolds. In this way one has obviated the difficulties encountered previously in the elimination of redundant coordinates (Lipkin *et al* 1955, Lipkin 1958a,b, 1960, Scheid and Greiner 1968, Eisenberg and Greiner 1970b, Villars and Cooper 1970, de Shalit and Feshbach 1974, Herold and Ruder 1979, Herold 1979).

The decomposition of \mathbb{R}^{3N} in (4.5) and T in (4.59) into a collective part defined on $\mathrm{GL}^+(3,\mathbb{R})$ (respectively $\mathrm{GL}^+(3,\mathbb{R})/\mathrm{SO}(3)$, see (4.58) and appendix 2) and an intrinsic part on $\mathrm{SO}(N)\backslash(\mathrm{SO}(3)\times\mathrm{SO}(N-3))$ (respectively $\mathrm{SO}(N)\backslash\mathrm{SO}(N-3)$) induces a corresponding decomposition of the N-particle Hilbert into irreducible subspaces defined on these manifolds. A complete set of functions for the intrinsic subspace is given by an irreducible unitary representation $\mathscr{D}^{\omega}_{\delta}$ of $\mathrm{SO}(N)$ restricted to subsets invariant under $\mathrm{SO}(3)\times\mathrm{SO}(N-3)$ (respectively $\mathrm{SO}(N-3)$) and reduced with respect to the various $\mathrm{SO}(N)$ subgroup chain‡. Together with functions (4.25) on $\mathrm{GL}^+(3,\mathbb{R})$ (respectively $\mathrm{GL}^+(3,\mathbb{R})/\mathrm{SO}(3)$)§ a complete set of functions for the N-particle Hilbert space is given by

$$\Psi_{M\mathcal{M}K\mathcal{K}\lambda\delta}^{L\mathcal{L}\omega} \equiv \mathscr{J}_{K\mathcal{K}\lambda}^{L\mathcal{L}}(I_{A})[\mathscr{D}_{MK}^{L}(r)\mathscr{D}_{\mathcal{M}\mathcal{K}}^{\mathcal{L}}(\bar{r}) + (-1)^{L+\mathcal{L}+K+\mathcal{H}}\mathscr{D}_{M-K}^{L}(r)\mathscr{D}_{\mathcal{M}-\mathcal{H}}^{\mathcal{L}}(\bar{r})]\mathscr{D}_{\delta}^{\omega}(R)$$

$$(4.60)$$

with $R \in SO(N) \setminus (SO(N-3))$ or respectively by

$$\Psi_{MMK\mathcal{H}\lambda\delta}^{L\mathscr{L}\omega} \equiv \mathscr{J}_{K\mathcal{H}\lambda}^{L\mathscr{L}}(I_{A})[\mathscr{D}_{MK}^{L}(r)\mathscr{D}_{\delta\mathcal{M}\mathcal{H}}^{\mathscr{L}}(\bar{R}) + (-1)^{L+\mathscr{L}+K+\mathscr{H}}\mathscr{D}_{M-K}^{L}(r)\mathscr{D}_{\delta\mathcal{M}-\mathscr{H}}^{\omega\mathscr{L}}(\bar{R})]$$
(4.61)

with $R \in SO(N) \setminus SO(N-3)$. The reduction of the N-particle Hilbert with respect to the group SO(N) allows one to take the Pauli principle and hence particle statistics fully into account. This circumstance arises from the well-known fact that the symmetric group S_N is a subgroup of O(N). Thus one is now enabled to construct from (4.60) or (4.61) orbital wavefunctions of the proper permutation symmetry and combine these with the spin-isospin functions of contragradient symmetry to obtain the total wavefunction. Detailed study of the relevant classification of the N-particle wavefunctions with respect to the unitary and symplectic groups and their subgroup chains including O(N) and S_N have been given by a number of authors (Vanagas and Kalinauskas 1974, Perkauskas *et al* 1975, Petrauskas and Sabalyauskas 1975, Asherova *et al* 1976, Vanagas 1976, 1977). Calculations for only light nuclei have so far been reported (Filippov and Maksimenko 1975, Filippov *et al* 1978, 1979).

Appendix 1. Vector fields for the normal space $(T_x \mathcal{M}_{G/H})^{\perp}$

From the r tangent vectors $(X_{\alpha})_x$ in (2.10) spanning the r-dimensional subspace $T_x \mathcal{M}_{G/H}$ of $T_x \mathbb{R}^{3N}$, one can easily construct a set of (3N-r) basis vectors $(Z_{\nu})_x$ for $(T_x \mathcal{M}_{G/H})^{\perp}$.

⁺ A minor difference arises from the centre-of-mass motion which we have ignored here. However, this is easily taken into account (cf Gulshani and Rowe 1976).

[‡] These functions generalise the usual spherical harmonics on SO(3)/SO(2) (see, for example, Vilenkin 1968, Strichartz 1975).

[§] As was pointed out in § 3.2 and will be shown in a subsequent work, more convenient collective basis functions are provided by an irreducible representation of the boson SU(6) group.

The result for r = 3N - 1, i.e. when $\mathcal{M}_{G/H}$ is a hypersurface in \mathbb{R}^{3N} , is well known (Synge and Schild 1961, Lovelock and Rund 1975). A generalisation of this result is immediate. Denote the components of Z_{ν} by Z_{ν}^{ni} and the pair indices *ni* by σ . Then

$$Z_1^{\sigma} \equiv \sum_{k=1}^{3N} \varepsilon_{\sigma\sigma_1\sigma_2\dots\sigma_r} X_1^{\sigma_1} X_2^{\sigma_2} \dots X_r^{\sigma_r}$$
(A.1.1)

where the permutation symbol ε is defined by $\varepsilon_{\sigma_1\sigma_2...\sigma_k} \equiv (0 \text{ if any two suffices are equal}; \pm 1 \text{ if the set } (\sigma_1, \sigma_2, \ldots, \sigma_k) \text{ is a selection from an even/odd permutation of the 3N integers } (1, 2, \ldots, N)). From (A1.1) it is evident that the vector field <math>Z_1 \equiv Z_1^{ni} \partial/\partial x^{ni}$ is orthogonal to X_{α} , i.e. $g(Z_1, X_{\alpha}) = 0$ for all α . From Z_1 and X_{α} we can now similarly construct Z_2 orthogonal to Z_1 and X_{α} and so on. Thus we obtain (3N - r) vector fields Z_{ν} with components

$$Z_{\nu}^{\sigma_{\nu}} \equiv \varepsilon_{\sigma_{\nu}\sigma_{\nu-1}\dots\sigma_{1}\omega_{1}\omega_{2}\dots\omega_{r}} Z_{\nu-1}^{\sigma_{\nu-1}} Z_{\nu-2}^{\sigma_{\nu-2}}\dots Z_{1}^{\sigma_{1}} X_{1}^{\omega_{1}} X_{2}^{\omega_{2}}\dots X_{r}^{\omega_{r}}$$
(A1.2)

for $\nu \ge 2$ where Z_1^{σ} is given in (A1.1)

Appendix 2. $G = GL^+(3, \mathbb{R}) \setminus SO(3)$ and G = SO(3)

To obtain the result (4.59) one may also identify the collective submanifold of \mathbb{R}^{3N} with the orbits of the left cosets $GL^+(3, \mathbb{R}) \setminus SO(3)$ as was done by Zickendraht (1971), Morinigo (1972), Dzyublik *et al* (1972), Filippov (1974), Ovcharenko (1976) and Vanagas (1977). In this case the intrinsic submanifold \mathcal{M}_{intr} in $\mathbb{R}^{3N} = \mathcal{M}_{GL/SO} \times \mathcal{M}_{intr}$ is identified with the Stiefel manifold S(3, N) of oriented orthonormal 3-frames in \mathbb{R}^N defined in § 4.3. SO(3) is then the isotropy subgroup of the action of $GL^+(3, \mathbb{R})$ on S(3, N) (cf (4.1) and (4.5)) because it maps one orthonormal 3-frame into another. From the diffeomorphism $S(3, N) = SO(N) \setminus SO(N-3)$ given in § 4.3 one then has the decomposition (cf (4.5)) $x^{ni} = g_{iA} \overline{R}_{An}$ with $g \in GL^+(3, \mathbb{R}) / SO(3)$ and $\overline{R} \in$ $SO(N) \setminus SO(N-3)$. But from (4.20) a representative coset in $GL^+(3, \mathbb{R}) / SO(3)$ is given by $g_{iA} = r_{Ai}S_A$. Therefore the above decomposition of \mathbb{R}^{3N} is given by

$$X^{ni} = r_{Ai} S_A \bar{R}_{An}$$
 $r \in SO(3)$ $S_A = (I_A/M)^{1/2}$. (A2.1)

In the corresponding decomposition $T_x \mathbb{R}^{3N} = T_x \mathcal{M}_{GL/SO} \oplus (T_x \mathcal{M}_{GL/SO})^c$ Dzyublik *et al* (1972), Filippov (1974), Ovcharenko (1976) and Vanagas (1977) made the identification $(T_x \mathcal{M}_{GL/SO})^c = T_x S(3, N)$ and obtained the result (4.59).

It is then interesting to apply the projection method to (A2.1). For this we have to make the choice $(T_x \mathcal{M}_{GL/SO})^c = (T_x \mathcal{M}_{GL/SO})^{\perp}$ and construct, from the general formula (3.4) and the vector fields L_A and t_A on $\mathcal{M}_{GL/SO}$ given in (4.21*a*) and (4.21*b*), the projector $\Gamma: T_x \mathbb{R}^{3N} \to T_x \mathcal{M}_{GL/SO}$. With respect to the basis $\{\partial/\partial x^{ni}\}$ for $T_x \mathbb{R}^{3N}$ we obtain

$$\Gamma_{ni,mj} \equiv \Gamma_{ni,mj}^{\text{rig}} + \Gamma_{ni,mj}^{\text{vib}} \tag{A2.2a}$$

where

$$\Gamma_{ni,mj}^{\text{vib}} \equiv (M/I_A) r_{Ai} r_{Aj} x^{mA} x^{nA} \qquad \Gamma_{ni,mj}^{\text{rig}} \equiv M X_k^{ni} \mathscr{G}_{kl}^{-1} X_l^{mj}.$$
(A2.2b)

In (A2.2b) \mathcal{I}^{-1} is the inverse of the rigid-body tensor \mathcal{I} defined by

$$\mathscr{I}_{kl} \equiv M X_l^{nl} X_k^{nl} = \delta_{lk} (\operatorname{Tr} Q) - Q_{lk} \qquad X_k^{nl} \equiv \varepsilon_{kll} x^{nl}.$$
(A2.3)

Q in (A2.3) is the mass quadrupole tensor in (4.7). Other quantities in (A2.2b) are given in (4.18) and (4.19). It is easy to show that Γ in (A2.2a) is a ($3N \times 3N$) symmetric and, since $\Gamma^{\text{rig}} \cdot \Gamma^{\text{vib}} = 0$, idempotent. Furthermore, rank $\Gamma = 6 = \dim (T_x \mathcal{M}_{\text{GL/SO}})$.

From (3.10) the decomposition of the particle momenta is then given by

$$p_{ni} \equiv -i\hbar \frac{\partial}{\partial x^{ni}} = p_{ni}^{\text{coll}} + p_{ni}^{\text{intr}}$$
(A2.4*a*)

where

$$p_{ni}^{intr} \equiv \Lambda_{ni,mj} p_{mj} \qquad p_{ni}^{coll} \equiv \Gamma_{ni,mj} p_{mj} \equiv p_{ni}^{rig} + p_{ni}^{vib} \qquad (A2.4b)$$

with

$$\Lambda_{ni,mj} \equiv \delta_{nm} \delta_{ij} - \Gamma_{ni,mj} \qquad p_{ni}^{\text{rig}} \equiv -i\hbar \varepsilon_{ijk} x^{nj} \mathcal{J}_{kl}^{-1} L_l \qquad (A2.4c)$$

and

$$p_{ni}^{\text{vib}} = -\frac{i\hbar M}{I_A} r_{Ai} x^{nA} t_A = -2i\hbar M R_{Ai} x^{nA} \frac{\partial}{\partial I_A}.$$
 (A2.4d)

The corresponding decomposition of the total kinetic energy is then given by (cf (3.13))

$$T = \frac{1}{2M} \sum_{n,i} p_{ni}^{2} = T_{\text{coll}} + T_{\text{intr}}$$
(A2.5*a*)

where

$$T_{\text{intr}} = \frac{1}{2M} p_{ni} \Lambda_{ni,mj} p_{mj} \qquad T_{\text{coll}} = \frac{1}{2M} p_{ni} \Gamma_{ni,mj} p_{mj} = T_{\text{rig}} + T_{\text{vib}} \qquad (A2.5b)$$

with

$$T_{\rm rig} = \frac{1}{2M} p_{ni} \Gamma_{ni,mj}^{\rm rig} p_{mj} = \frac{1}{2} L_i \mathscr{I}_{ij}^{-1} L_j$$
(A2.5c)

and

$$T_{\rm vib} \equiv \frac{1}{2M} p_{ni} \Gamma^{\rm vib}_{ni,mj} p_{mj} = -2\hbar^2 \sum_{A=1}^3 I_A \left[\frac{\partial^2}{\partial I_A^2} + \left(\frac{N-2}{I_A} + \sum_{B \neq A}^3 \frac{1}{I_A - I_B} \right) \frac{\partial}{\partial I_A} \right].$$
(A2.5d)

In deriving (A2.5d) we have used the result

$$\sum_{n,i} \frac{\partial}{\partial x^{ni}} (r_{Ai} x^{nA}) = N - 2 + \sum_{B \neq A}^{3} \frac{I_A}{I_A - I_B}$$

which can be derived from a previous result (Gulshani and Rowe 1976, equation (2.18)).

We observe that T_{vib} in (A2.5*d*) is identical to that in (4.24*b*). But the rotational kinetic energy T_{rig} in (A2.5*c*) is that of the rigid body and clearly differs from T_{rot} in (4.24*c*). In fact, T_{rot} is expressible as the sum of T_{rig} and other terms involving both L_A and \mathcal{L}_A (Gulshani and Rowe 1976). These latter terms must, therefore, be included in T_{intr} in (A2.5*b*). Thus an appropriate set of intrinsic vector fields may now be seen to be some vector fields on SO(3N) \supset SO(3) \times SO(N) so as to involve both L_A and J_{nm} in (4.26). We have not yet been able to express T_{intr} in terms of such vector fields and obtain the result (4.59) and thereby establish the equivalence of the approach in this appendix and that of § 4. Similar difficulty is encountered when we consider the

rotational motion. For this motion the collective submanifold of \mathbb{R}^{3N} is identified with the orbits of SO(3). The corresponding projector and the decompositions of the momenta and the kinetic energy are easily discernible in equations (A2.2), (A2.4) and (A2.5) (cf Gulshani 1981).

Appendix 3. The source of non-integrability

We have seen in § 4.3 that the Grassman manifold of 3-frames G(3, N) is not an integral manifold of the distribution determined by the normal space $(T_x \mathcal{M}_{GL})^{\perp}$, i.e. $(T_x \mathcal{M}_{GL})^{\perp} \neq T_x G(3, N)$. Here we show that if we require $(T_x \mathcal{M}_{GL})^{\perp} = T_x G(3, N)$ as was done before (Gulshani and Rowe 1976), then every coordinate system on G(3, N) is non-integrable on \mathbb{R}^{3N} . Let $\{g_{ij}\}$ and $\{\xi^{\sigma} | 1 \leq \sigma \leq 3N - 9\}$ be a system of coordinates on $GL^+(3, \mathbb{R})$ and G(3, N) respectively. Then equation (4.5) becomes

$$x^{n} = g_{i\alpha} R_{\alpha n}(\xi^{\sigma}). \tag{A3.1}$$

Clearly the infinitesimal operators t_{ij} of $\operatorname{GL}^+(3, \mathbb{R})$ do not act on $R_{\alpha n} \in \operatorname{SO}(N) \setminus (\operatorname{SO}(3) \times \operatorname{SO}(N-3))$. It then follows that, in the chain-rule expansion

$$\frac{\partial}{\partial x^{ni}} = \frac{\partial g_{lk}}{\partial x^{ni}} \frac{\partial}{\partial g_{lk}} + \frac{\partial \xi^{\sigma}}{\partial x^{ni}} \frac{\partial}{\partial \xi^{\sigma}}$$
(A3.2)

and hence

$$t_{ij} \equiv x^{ni} \frac{\partial}{\partial x^{nj}} = x^{ni} \frac{\partial g_{lk}}{\partial x^{nj}} \frac{\partial}{\partial g_{lk}} + x^{ni} \frac{\partial \xi^{\sigma}}{\partial x^{nj}} \frac{\partial}{\partial \xi^{\sigma}}$$

we must have

$$x^m \partial \xi^\sigma / \partial x^m = 0$$
 for all *i*, *j* and σ . (A3.3)

Now we can relate $\partial \xi^{\sigma} / \partial x^{n}$ to $\partial x^{n} / \partial \xi^{\sigma}$ by using the intrinsic metric as follows (Gulshani and Rowe 1976, appendices I and III): in terms of an arbitrary complete set of coordinates $\{\eta^{\nu} | 1 \le \nu \le 3N\}$ on \mathbb{R}^{3N} the metric g on \mathbb{R}^{3N} is defined by the arc length

$$\mathrm{d}s^2 \equiv \mathrm{d}x^{ni} \,\mathrm{d}x^{ni} = \frac{\partial x^{ni}}{\partial \eta^{\nu}} \frac{\partial x^{ni}}{\partial \eta^{\mu}} \,\mathrm{d}\eta^{\nu} \,\mathrm{d}\eta^{\mu} \equiv g_{\nu\eta} \,\mathrm{d}\eta^{\nu} \,\mathrm{d}\eta^{\mu}.$$

Since $\{\eta^{\nu}\}$ is a complete set we have

$$\frac{\partial x^{n_i}}{\partial \eta^{\nu}} \frac{\partial \eta^{\nu}}{\partial x^{m_j}} = \delta_{nm} \delta_{ij}$$

and therefore

$$g_{\nu\mu}\frac{\partial \eta^{\mu}}{\partial x^{nl}} = \frac{\partial x^{nl}}{\partial \eta^{\nu}}.$$
(A3.4)

Now the requirement that $T_x \mathcal{M}_{GL}$ be orthogonal to $T_x G(3, N)$, i.e. $(T_x \mathcal{M}_{GL})^{\perp} = T_x G(3, N)$, implies that the metric g be block diagonal in terms of the coordinates $\{g_{ij}, \xi^{\sigma}\}$, i.e.

$$g = \left(\frac{g_{ij}}{0} \middle| \frac{0}{g_{\sigma\bar{\sigma}}}\right)$$

(Gulshani and Rowe 1976, appendix III). It then follows from equation (A3.4) that

$$g_{\sigma\bar{\sigma}}\frac{\partial\xi^{\bar{\sigma}}}{\partial x^{ni}} = \frac{\partial x^{ni}}{\partial\xi^{\bar{\sigma}}}.$$
(A3.5)

Multiplying (A3.3) by $g_{\sigma\sigma}$, summing over σ and using (A3.5), we obtain the constraint equations

$$x^{ni}\frac{\partial x^{nj}}{\partial \xi^{\sigma}} \equiv 0. \tag{A3.6}$$

Equation (A3.6) is made up of two parts: a symmetric part

$$x^{ni}\frac{\partial x^{nj}}{\partial \xi^{\sigma}} + x^{nj}\frac{\partial x^{ni}}{\partial \xi^{\sigma}} = \frac{\partial}{\partial \xi^{\sigma}}(x^{ni}x^{nj}) = 0$$
(A3.7)

and a skew symmetric part

$$x^{ni}\frac{\partial x^{nj}}{\partial \xi^{\sigma}} - x^{nj}\frac{\partial x^{ni}}{\partial \xi^{\sigma}} = 0.$$
 (A3.8)

Constraint equations (A3.7) and (A3.8) are separately integrable. (A3.7) is clearly integrable by virtue of (4.5) and (4.7) and, contrary to the assumption made by Rowe (1970), (A3.8) has a solution given by

$$\frac{\partial x^{ni}}{\partial \xi^{\sigma}} = C_{\sigma}^{ni} x^{ni}$$

with C_{σ}^{ni} being arbitrary functions of x^{ni} . However, (A3.7) and (A3.8) are not compatible constraints with the result that (A3.6) are not integrable as we now show.

Differentiating (A3.8) with respect to x^{mk} , we obtain

$$0 = \delta_{ik} \frac{\partial x^{mj}}{\partial \xi^{\sigma}} - \delta_{jk} \frac{\partial x^{mi}}{\partial \xi^{\sigma}} + x^{ni} \frac{\partial^2 x^{nj}}{\partial x^{mk} \partial \xi^{\sigma}} - x^{nj} \frac{\partial^2 x^{ni}}{\partial x^{mk} \partial \xi^{\sigma}}.$$
 (A3.9)

To show that the last two terms in (A3.9) cancel each other consider

$$x^{ni} \frac{\partial^2 x^{nj}}{\partial x^{mk} \partial \xi^{\sigma}} = x^{ni} \frac{\partial \xi^{\nu}}{\partial x^{mk}} \frac{\partial^2 x^{nj}}{\partial \xi^{\nu} \partial \xi^{\sigma}} + \frac{\partial g_{i\alpha}}{\partial x^{mk}} x^{ni} \frac{\partial R_{\alpha n}}{\partial \xi^{\sigma}}$$
(A3.10)

where we have used (A3.2) and (4.5). Now the last term in (A3.10) vanishes by virtue of (A3.6). Assuming that x^{ni} are differentiable functions of ξ^{σ} so that we can interchange the order of differentiation with respect to ξ^{ν} and ξ^{σ} in the first term on the right-hand side of equation (A3.10), we obtain, with repeated use of (A3.6),

$$x^{ni}\frac{\partial^{2}x^{nj}}{\partial x^{mk}\partial\xi^{\sigma}} = x^{ni}\frac{\partial\xi^{\nu}}{\partial x^{mk}}\frac{\partial^{2}x^{nj}}{\partial\xi^{\nu}\partial\xi^{\sigma}} = x^{ni}\frac{\partial\xi^{\nu}}{\partial x^{mk}}\frac{\partial^{2}x^{nj}}{\partial\xi^{\sigma}\partial\xi^{\nu}}$$
$$= -\frac{\partial\xi^{\nu}}{\partial x^{mk}}\frac{\partial x^{ni}}{\partial\xi^{\sigma}}\frac{\partial x^{nj}}{\partial\xi^{\nu}} = \frac{\partial\xi^{\nu}}{\partial x^{mk}}x^{nj}\frac{\partial^{2}x^{ni}}{\partial\xi^{\nu}\partial\xi^{\sigma}} = x^{nj}\frac{\partial^{2}x^{ni}}{\partial x^{mk}\partial\xi^{\sigma}}$$
(A3.11)

where the chain rule (A3.2) is used again to obtain the last equality in (A3.11). From equations (A3.11) and (A3.9) we then obtain the result

$$0 = \delta_{ik} \frac{\partial x^{mj}}{\partial \xi^{\sigma}} - \delta_{jk} \frac{\partial x^{mi}}{\partial \xi^{\sigma}}$$

which implies that

$$\partial x^{m_i} / \partial \xi^{\sigma} = 0$$
 for all m, j and σ . (A3.12)

Conditions (A3.12) imply that x^{m_i} must be independent of ξ^{σ} (i.e. frozen intrinsic structure) for the constraint equations (A3.6) to be integrable. Otherwise the assumption of differentiability of x^{n_i} with respect to ξ^{σ} used in (A3.11) is false and we have the non-integrability condition:

 $\frac{\partial^2 x^{n_i}}{\partial \xi^{\nu} \partial \xi^{\sigma}} \neq \frac{\partial^2 x^{n_i}}{\partial \xi^{\sigma} \partial \xi^{\nu}}.$ (A3.13)

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