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Invariant manifolds and collective coordinates

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Abstract

We introduce suitable coordinate systems for interacting many-body systems with invariant manifolds. These are Cartesian in coordinate and momentum space and chosen such that several components are identically zero for motion on the invariant manifold. In this sense these coordinates are collective. We make a connection to Zickendraht's collective coordinates and present certain configurations of few-body systems where rotations and vibrations decouple from single-particle motion. These configurations do not depend on details of the interaction.

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1. Introduction

Dynamical systems with invariant manifolds in phase space have been the subject of ongoing research in recent years. Many authors have considered the case of two or more coupled identical systems that are chaotic [1–7]. On invariant manifolds the subsystems display identical or synchronized motion. This synchronized behaviour can be maintained for long times if the motion is stable in transverse directions of the manifold.

Many-particle systems like atomic nuclei display synchronized or collective behaviour, too, even though their Hamiltonians are probably largely chaotic. It is interesting to relate this kind of collective motion to the synchronized motion on invariant manifolds. This idea is based on the fact that a rotationally invariant system of identical interacting particles possesses low-dimensional invariant manifolds in classical phase space [8]. On invariant manifolds many particles participate in synchronized motion and decouple from more complex single-particle behaviour. The importance of a given invariant manifold depends crucially on its stability properties. If the manifold under consideration is sufficiently stable in transverse directions, the quantum system may exhibit wavefunction scarring [9–11] or display a strong revival for wavepackets localized to the vicinity of the manifold [12]. These findings may be directly

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associated with the slow decay of collective motion due to the coupling between collective and single-particle motion.

It is thus of interest to introduce coordinates that are particularly adapted to an invariant manifold. The coordinates along the manifold correspond to collective degrees of freedom while those in transverse direction can be identified with single-particle degrees of freedom. Such coordinate systems may be useful for several applications. We have in mind (i) the problem of damping and dissipation of collective excitations and the interplay of collective and chaotic motion in atomic nuclei [13–20], which is often addressed in the framework of single-particle motion in a time-dependent mean field; (ii) multi-particle fragmentation of atoms at the threshold which evolves over highly symmetric configurations corresponding to invariant manifolds [9, 21]; (iii) the structural stability of invariant manifolds [22] and (iv) the structure of intrinsic coordinates in many-body systems [23].

There is a traditional way to introduce collective and single-particle coordinates in interacting many-body systems. Aiming at the description of nuclear vibrations and rotations, Zickendraht [24] introduced a system of collective coordinates in a self-bound many-body system. Three of these coordinates describe the centre of mass motion, and six collective degrees of freedom govern the dynamics of the inertia ellipsoid. The remaining coordinates are of single-particle nature. We shall establish the relation of coordinates of invariant manifolds to those defined by Zickendraht. Furthermore we shall show that more complicated collective motion, e.g. shearing modes, can also be described in this framework.

This paper is divided as follows. In the next two sections we introduce suitable coordinate systems for interacting many-body systems with invariant manifolds. We give a construction recipe and present a detailed example calculation. As an application we give a potential expansion around an invariant manifold and discuss stability properties. In section 4 we make a connection with the Zickendraht coordinates. We present examples where the motion of the inertia ellipsoid corresponds to the motion on an invariant manifold. For such initial conditions the traditional collective motion decouples completely from the single-particle degrees of freedom. We also find that collective coordinates as defined here are capable of other types of motion. Therefore we finally discuss how motion on or near such invariant manifolds could be interpreted as collective motion of a system.

2. Coordinates for invariant manifolds

In this section we present a transformation from Cartesian single-particle coordinates in position and momentum space to Cartesian coordinates that are adapted to invariant manifolds. The new coordinates consist of ‘collective coordinates’ that govern the motion on the invariant manifold and of coordinates transversal to this manifold that represent the single-particle aspects.

Consider rotationally invariant systems of N identical particles in d spatial dimensions ($d = 2$ or 3). The Hamiltonian is invariant under both the action of the rotation group $O(d)$ and the group of permutations S_N . One may now take a finite subgroup $\mathcal{G} \subset O(d)$ with elements g and properly chosen permutations $P(g)$ such that

$$gP^{-1}(g)(\vec{p}, \vec{q}) = (\vec{p}, \vec{q}) \quad \forall g \in \mathcal{G} \quad \vec{p} \equiv (p_1, \dots, p_{Nd}) \quad \vec{q} \equiv (q_1, \dots, q_{Nd}) \quad (1)$$

for points (\vec{p}, \vec{q}) on a manifold which will be invariant under any Hamiltonian with the $O(d) \times S_N$ symmetry, because the pairs $(g, P^{-1}(g))$ form a subgroup of the symmetry group. In this subgroup, which is isomorphic to \mathcal{G} , permutations cancel rotations when acting on the manifold.

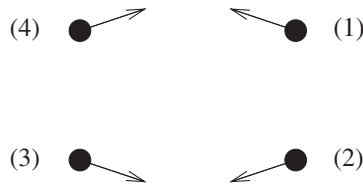


Figure 1. Collective configuration on invariant manifold. Positions are indicated by filled circles and momenta by arrows.

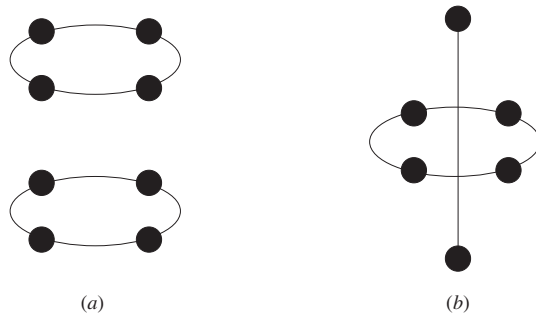


Figure 2. Configurations of eight (a) or six (b) particles in three dimensions that correspond to invariant manifolds. Positions are indicated by filled circles.

Figure 1 shows a configuration of four particles in two spatial dimensions that corresponds to a point on an invariant manifold of the type defined above. The operations of elements from the discrete symmetry group $\mathcal{G} = C_{2v}$ can be undone by suitable permutations of particles. This leads to a collective motion with two degrees of freedom which we shall identify with vibrations.

Figure 2 shows two spatial configurations of eight 2(a) and six 2(b) particles, respectively, which display a D_{4h} symmetry. If initial momenta display the same symmetry the motion on the invariant manifold will have two degrees of freedom. For eight particles the radii of the two circles will oscillate synchronously, and the two circles will vibrate against each other. For the six particles we will have a vibration of the radius of the circle and of the two particles along the vertical axis. We may choose initial momenta to reduce the symmetry group to C_{4h} , which will allow rotations around the vertical axis and thus add an additional degree of freedom. For eight particles we could alternatively choose initial conditions that are limited to a D_4 symmetry. Besides the vibrations discussed above this would allow for a shearing motion of the two circles thus yielding again three degrees of freedom. We could also reduce the fourfold rotation axis to a twofold one and obtain D_{2h} , D_2 or C_{2v} as remaining symmetry groups yielding more collective degrees of freedom. Adding two particles symmetrically onto the principal axis of rotation would also increase the number of degrees of freedom by one. Different reductions of symmetry will yield different invariant manifolds with varying degrees of freedom. We will see this exemplified by explicit construction of coordinates.

We may use the definition (1) directly for the construction of coordinate systems where invariant manifolds correspond to coordinate axis or planes, i.e. non-collective coordinates vanish for motion on the invariant manifold. To this purpose we consider the many-body system in Cartesian coordinates in momentum and position space. In what follows we will introduce orthogonal transformations in configuration space only; momenta will be subject to the same transformation.

In a Cartesian coordinate system each element $g \in \mathcal{G}$ and each permutation $P(g)$ can be represented by an orthogonal matrix M_g and P_g of dimension Nd . It is clear that the products $M_g P_g^T$ form a matrix group \mathcal{H} that acts onto position and momentum space, respectively. The construction of the coordinate system is now straightforward. Every vector \vec{p} and \vec{q} may be expanded in basis vectors of the irreducible representations (IRs) of \mathcal{H} by means of projectors [25].

$$\Pi_\nu = \sum_{g \in \mathcal{G}} \chi_g^{(\nu)} M_g P_g^T. \quad (2)$$

Here $\chi_g^{(\nu)}$ denotes the character of g in the ν th IR. Similar formulae hold for momentum space. The projection onto the identical IR defines the invariant manifold. Note that the identical representation is one dimensional while the invariant manifolds of interest typically have higher dimensionality. This dimensionality depends both on the group \mathcal{G} and on the specific configuration chosen among all configurations invariant under \mathcal{G} . To determine the dimension in general we would need induced representations to identify the number of independent invariant vectors, but in practice the construction of all independent vectors by projection technique seems to be unproblematic as we shall see in the example.

A comment on the rotation symmetry is in order. Like any Cartesian coordinates, the coordinates introduced in this paper do not explicitly reflect the invariance under rotations. Acting on an invariant manifold, rotations generate a continuous family of equivalent manifolds. Our coordinates, however, single out one particular manifold. For quantum systems, the rotation operator may easily be constructed and used for projection onto subspaces of definite angular momentum.

3. A simple example

We now illustrate the proposed construction explicitly for four particles in two dimensions and a quartic potential, considering the invariant manifold shown in figure 1. We shall also expand the potential near the invariant manifold to second order in the transversal coordinates.

The invariant manifold is defined by those points which are invariant under $\mathcal{H} = \{E, \sigma_x P_{(12)(34)}, \sigma_y P_{(14)(23)}, C_2 P_{(13)(24)}\}$, where E denotes the identity, P a permutation of particles as indicated, σ a reflection at the axis indicated and C_2 a rotation by π about the origin. Thus, $\mathcal{H} = C_{2v}$ with four IRs labelled by $\nu = A_1, B_1, A_2, B_2$ [25]. Let $\vec{q} = (x_1, x_2, x_3, x_4, y_1, y_2, y_3, y_4)$ denote a coordinate vector in position space (x_i, y_i denote the coordinates of the i th particle). We have

$$\begin{aligned} E \vec{q} &= (x_1, x_2, x_3, x_4, y_1, y_2, y_3, y_4) \\ \sigma_x P_{(12)(34)} \vec{q} &= (x_2, x_1, x_4, x_3, -y_2, -y_1, -y_4, -y_3) \\ C_2 P_{(13)(24)} \vec{q} &= (-x_3, -x_4, -x_1, -x_2, -y_3, -y_4, -y_1, -y_2) \\ \sigma_y P_{(14)(23)} \vec{q} &= (-x_4, -x_3, -x_2, -x_1, y_4, y_3, y_2, y_1). \end{aligned}$$

Using the character table of C_{2v} [25] and the projectors (2) one constructs the following basis vectors corresponding to the IR labelled by

$$\begin{aligned} A_1: \quad e'_1 &= (1, 1, -1, -1, 0, 0, 0, 0)/2 & e'_2 &= (0, 0, 0, 0, 1, -1, -1, 1)/2 \\ B_1: \quad e'_3 &= (1, 1, 1, 1, 0, 0, 0, 0)/2 & e'_4 &= (0, 0, 0, 0, 1, -1, 1, -1)/2 \\ A_2: \quad e'_5 &= (1, -1, -1, 1, 0, 0, 0, 0)/2 & e'_6 &= (0, 0, 0, 0, 1, 1, -1, -1)/2 \\ B_2: \quad e'_7 &= (1, -1, 1, -1, 0, 0, 0, 0)/2 & e'_8 &= (0, 0, 0, 0, 1, 1, 1, 1)/2. \end{aligned}$$

The vectors associated with the identical IR A_1 span the two-dimensional invariant manifold and the vectors associated with the IRs B_1, A_2, B_2 span the transverse directions. It is straightforward to compute the orthogonal transformation matrix from the basis vectors of the IRs.

To illustrate the example and to further demonstrate the usefulness of the newly introduced coordinate system we want to consider the the interacting four-body system with Hamiltonian

$$H = \sum_{i=1}^4 ((p_{x_i}^2 + p_{y_i}^2)/2 + 16(x_i^2 + y_i^2)^2) - \sum_{i < j} [(x_i - x_j)^2 + (y_i - y_j)^2]^2. \quad (3)$$

This Hamiltonian has been studied previously [12]. In particular, the stability of the invariant manifold displayed in figure 1 has been studied by computing the full phase space monodromy matrix of several periodic orbits that are inside the invariant manifold. It was found that several orbits are linearly stable in transverse directions or possess rather small stability exponents. Qualitatively, this may also be understood by studying the Hamiltonian (3) close to the invariant manifold. We therefore expand the potential of Hamiltonian (3) to second order in the transverse directions labelled by $(\epsilon_1, \dots, \epsilon_6)$ while keeping the full dependence of the coordinates (x, y) inside the invariant manifold. One obtains the quadratic form $\vec{\epsilon}^T \mathbf{V} \vec{\epsilon}$ where

$$\mathbf{V} = \begin{bmatrix} 12x^2 + 4y^2 & 0 & 0 & 16xy & 0 & 0 \\ 0 & 12x^2 & 0 & 0 & 8xy & 0 \\ 0 & 0 & 24x^2 + 8y^2 & 0 & 0 & 16xy \\ 16xy & 0 & 0 & 8x^2 + 24y^2 & 0 & 0 \\ 0 & 8xy & 0 & 0 & 12y^2 & 0 \\ 0 & 0 & 16xy & 0 & 0 & 4x^2 + 12y^2 \end{bmatrix}.$$

Application of the Sylvester criterion shows that the matrix \mathbf{V} is positive definite for $x, y \neq 0$. Five of the eigenvalues of \mathbf{V} vanish only at the origin $x = y = 0$; one eigenvalue vanishes for $x = 0$ or $y = 0$. Thus, instability may only occur along the coordinate axes of the invariant manifold. Though the expansion of a potential around an invariant manifold is no substitute for the computations of Lyapunov exponents or monodromy matrices, it is a first step when estimating stability properties of such manifolds.

4. Zickendraht's coordinates and invariant manifolds

Almost 30 years ago Zickendraht [24] introduced a set of collective coordinates to describe nuclear vibrations and rotations, as well as their coupling with single-particle motion. We shall discuss to what extent these coordinates correspond to the ones we introduced in the previous sections. On one hand this will allow us to identify certain vibrational modes of a many-body system with invariant manifolds. On the other hand we shall also see that our procedure proposes collective movements that are not of the type described easily in Zickendraht's coordinates.

Following Zickendraht [24] we write the coordinates \vec{r}_i of the i th particle in the centre of mass system as

$$\vec{r}_i = s_{i1} \vec{y}_1 + s_{i2} \vec{y}_2 + s_{i3} \vec{y}_3 \quad i = 1, \dots, N \quad (4)$$

where the \vec{y}_i span the inertia ellipsoid and s_{ik} are non-collective coordinates which for simplicity we shall call single-particle coordinates. The newly introduced coordinates \vec{y}_i and s_{ij} are not independent. The constraints are

$$\begin{aligned} \vec{y}_i \cdot \vec{y}_j &= y_i y_j \delta_{ij} & i, j &= 1, 2, 3 \\ \sum_{i=0}^N s_{ij} &= 0 & j &= 1, 2, 3 \\ \sum_{i=0}^N s_{ij} s_{ik} &= \delta_{jk} & j, k &= 1, 2, 3. \end{aligned}$$

The first six equations ensure the orthogonality and normalization of the principal axis of the inertia ellipsoid whereas the next three equations fix the origin at the centre of mass system. The last six equations are orthogonality relations of the single-particle coordinates. In the centre of mass system, one may therefore characterize the N -body system by its inertia ellipsoid (e.g.

three Euler angles of the principle axis and three moments of inertia) and $3N - 9$ single-particle coordinates. The moments of inertia I_i are related to the coordinates y_i by

$$I_1 = m(y_2^2 + y_3^2) \quad I_2 = m(y_1^2 + y_3^2) \quad I_3 = m(y_1^2 + y_2^2) \quad (5)$$

where m denotes the mass of the particles.

It is interesting to determine those configurations where the motion of the many-body system may be described in terms of the collective coordinates y_i only. While such motion would be restricted to *some* invariant manifold in phase space it would not obviously be one of those defined by equation (1). We may however determine invariant manifolds (1) such that the motion on the manifold changes only the inertia ellipsoid of the system and hence may be described entirely by Zickendraht's collective coordinates y_i . Two necessary conditions for this situation are easily stated. First, the number of coordinates on such an invariant manifold may not exceed six in the general case and three in the case of pure vibrations. Second, every motion on such an invariant manifold has to change the inertia ellipsoid of the many-body system.

For simplicity let us start with a system of four particles in two spatial dimensions and the invariant manifold displayed in figure 1, i.e.

$$\vec{r}_1 = \begin{bmatrix} x \\ y \end{bmatrix} \quad \vec{r}_2 = \begin{bmatrix} x \\ -y \end{bmatrix} \quad \vec{r}_3 = \begin{bmatrix} -x \\ -y \end{bmatrix} \quad \vec{r}_4 = \begin{bmatrix} -x \\ y \end{bmatrix}$$

and the momenta chosen by replacing $x \rightarrow p_x, y \rightarrow p_y$. Computation of the moments of inertia yield the collective Zickendraht coordinates $y_1 = 2x, y_2 = 2y$. On the invariant manifold the remaining coordinates are given by $s_{11} = s_{12} = s_{21} = -s_{22} = -s_{31} = -s_{32} = -s_{41} = s_{42} = 1/2$. This shows that every motion on the invariant manifold only changes the moments of inertia and therefore decouples from the single-particle motion.

We next consider the example of an eight-body system in three dimensions. Let

$$\vec{r}_1 = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad \vec{r}_2 = \begin{bmatrix} -y \\ x \\ z \end{bmatrix} \quad \vec{r}_3 = \begin{bmatrix} -x \\ -y \\ z \end{bmatrix} \quad \vec{r}_4 = \begin{bmatrix} y \\ -x \\ z \end{bmatrix} \quad \vec{r}_{4+i} = \vec{r}_i (z \leftrightarrow -z) \quad (6)$$

denote a configuration restricted to the invariant manifold displayed in figure 2(a) with C_{4h} symmetry. (The momenta are chosen by replacing $x \rightarrow p_x, y \rightarrow p_y, z \rightarrow p_z$ in equation (6).) The moments of inertia are $I_1 = I_2 = 4m(x^2 + y^2) + 8mz^2, I_3 = 8m(x^2 + y^2)$ and yield collective coordinates (5) $y_1^2 = y_2^2 = 4(x^2 + y^2), y_3^2 = 8z^2$. Since the inertia ellipsoid is symmetric we have a freedom in choosing two of its principle axes. Using

$$\vec{y}_1 = 2 \begin{bmatrix} x \\ y \\ 0 \end{bmatrix} \quad \vec{y}_2 = 2 \begin{bmatrix} -y \\ x \\ 0 \end{bmatrix} \quad \vec{y}_3 = \sqrt{8} \begin{bmatrix} 0 \\ 0 \\ z \end{bmatrix}$$

one obtains constant single-particle coordinates $s_{11} = -s_{31} = s_{51} = -s_{71} = s_{22} = -s_{42} = s_{62} = -s_{82} = 1/2, s_{13} = s_{23} = s_{33} = s_{43} = -s_{53} = -s_{63} = -s_{73} = -s_{83} = 1/\sqrt{8}$ for the motion on the invariant manifold. Thus, the single-particle motion decouples from the collective motion on the invariant manifold. Similar results hold for the six-particle configuration displayed in figure 2.

It is also instructive to consider an example which goes beyond Zickendraht's collective coordinates. The configuration

$$\vec{r}_1 = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad \vec{r}_2 = \begin{bmatrix} -y \\ x \\ z \end{bmatrix} \quad \vec{r}_3 = \begin{bmatrix} -x \\ -y \\ z \end{bmatrix} \quad \vec{r}_4 = \begin{bmatrix} y \\ -x \\ z \end{bmatrix}$$

$$\vec{r}_5 = \begin{bmatrix} x \\ -y \\ -z \end{bmatrix} \quad \vec{r}_6 = \begin{bmatrix} y \\ x \\ -z \end{bmatrix} \quad \vec{r}_7 = \begin{bmatrix} -x \\ y \\ -z \end{bmatrix} \quad \vec{r}_8 = \begin{bmatrix} -y \\ -x \\ -z \end{bmatrix}$$

displays D_4 symmetry and differs from configuration (6) by a shearing motion. As in the previous example, the moments of inertia are given by $I_1 = I_2 = 4m(x^2 + y^2) + 8mz^2$, $I_3 = 8m(x^2 + y^2)$ and the ellipsoid of inertia is symmetric. However, no choice of the principal axis allows us to fulfill equations (4) with *constant* single-particle coordinates s_{ij} . Therefore, single-particle degrees of freedom depend on collective degrees of freedom and a decoupling does not exist using Zickendraht's coordinate system. A decoupling is obtained by using the coordinates introduced in this work. However, the collective motion on the appropriate invariant manifold does not correspond to pure vibrations or rotations of the inertia ellipsoid. These findings are interesting e.g. in relation with the magnetic dipole mode in nuclei [26] since this type of collective behaviour is associated with a shearing motion. Interest in collective shearing modes has recently revived due to new experiments of electron scattering on heavy, deformed nuclei [27].

5. Discussion

We constructed an orthogonal transformation that maps the Cartesian single-particle coordinates of a many-body system to a new Cartesian coordinate system that distinguishes collective and single-particle motion. The collective degrees of freedom govern the motion that is restricted to a low-dimensional invariant manifold and are decoupled from single-particle degrees of freedom on this manifold. We have demonstrated that there are several configurations of few-body systems, where the motion on the invariant manifold corresponds to a vibration or rotation and may be described in terms of Zickendraht's collective coordinates, but differs when the collective motion goes beyond that. These results are independent of the details of the Hamiltonian of the N -body system, and are entirely determined by rotational and permutational symmetry.

Using the results of this paper as well as those of [11, 12] we can draw the following picture: first it is possible that an invariant manifold is spanned exactly by the vibrational and rotational modes of a few-body system; second such manifolds may be stable or have small instability exponents in transversal directions; third the revival probabilities of wavepackets launched on such manifolds are large; last, as a conclusion of these points we may have a collective motion near the manifold whose damping is characterized by the decay rate in the transversal direction. We also found that there may be other collective motions; this was displayed in an example of shearing motion. The coincidence of Zickendraht coordinates with our collective coordinates depends on particle numbers; typically they do not span an invariant manifold. This confirms the well known fact that in general the collective motion in these coordinates does not separate rigorously, but only in some adiabatic approximation.

As we have found more general invariant configurations, which in turn induce collective coordinates, we may hope that these are useful for approximate considerations for larger particle numbers that do include the corresponding invariant manifold in a non-trivial fashion. We may finally note that the projection method proposed for the construction of coordinates for invariant manifolds induced by symmetry groups is not restricted to systems with rotation and permutation symmetry. Whenever the system has manifolds that are transformed pointwise into themselves under some subgroup of the symmetry group the method applies. An obvious candidate is a molecule in the Born–Oppenheimer approximation where $O(3)$ is replaced by a point group.

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