All transformations of coordinates that separate the center of mass kinetic energy, their group structure and geometry

2010 J. Phys. A: Math. Theor. 43 065301

(http://iopscience.iop.org/1751-8121/43/6/065301)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **43** (2010) 065301 (9pp) doi:10.1088/1751-8113/43/6/065301

All transformations of coordinates that separate the center of mass kinetic energy, their group structure and geometry

L Fortunato

ECT*, Strada delle Tabarelle 286, I-38050 Villazzano (TN), Italy

E-mail: fortunato@ect.it and fortunat@pd.infn.it

Received 13 October 2009, in final form 10 December 2009
Published 19 January 2010
Online at stacks.iop.org/JPhysA/43/065301

Abstract

The most general transformations of coordinates that allow for the exact separation of the kinetic energy operator of a quantum many-body system into total center of mass kinetic energy and internal kinetic energy are found and discussed. It is found (i) that the suitable transformations, depending on the number of particles, have a certain number of free parameters and this allows for the generalization of the Jacobi coordinates to a much larger class of coordinates with the same properties and (ii) that there is a new, uncommon, additive group structure hidden in the transformation matrices that is connected to certain geometric properties of the set of coordinates.

PACS numbers: 02.10.Yn, 02.20.−a, 24.10.Cn

1. Introduction

The kinetic energy operator of a set of particles in quantum mechanics depends upon the Laplacian of the coordinates:

$$T = \sum_{1}^{n} T_i = \sum_{1}^{n} -\frac{\hbar^2}{2m_i}\nabla^2_{\vec{r}_i} \tag{1}$$

where the summation is extended over all particles $i = \{1, \ldots, n\}$ with position vectors $\vec{r}_i$. The Hamiltonian of the system depends on this operator and in the study of the internal excitations of a quantum system we are faced with the fundamental problem of eliminating the kinetic energy of the center of mass from the total Hamiltonian. Several transformations of coordinates, techniques and methods exist to accomplish this task [1, 2]; I would like to mention the transformation to Jacobi coordinates that singles out the center of mass energy [3]. This is a crucial step in atomic, molecular and nuclear physics. The general idea behind this is the following conversion:

$$T = \sum_{1}^{n} T_i \longrightarrow \sum_{1}^{n-1} T'_i + \frac{\vec{P}^2}{2M} \tag{2}$$

where $\vec{P} = (1/n)\sum_1^n \vec{p}_n$ is the linear momentum of the center of mass of the system with total mass $M = \sum_1^n m_i$.

It is generally recognized that there are several sets of Jacobi coordinates that accomplish this task [1] and that not only can one change the labeling of particles but one can also change the order in which particles are grouped together, thus generating a large number of possible sets of Jacobi coordinates. Several authors have studied the problem of transformations of coordinates for various reasons or applications, and they have even included masses (see [4], where a matrix very similar to the ones I derive in the following appears), but to my knowledge the most general conditions under which one can expect center of mass separation to occur have not yet been thoroughly worked out. I must therefore apologize to all those authors whose researches are not cited in the present paper, but my intention is to look at the problem from a wider angle, and specific applications, although arguably very important, are not referenced. In addition, the present analysis reveals an uncommon group structure hidden in the transformation matrices that has a connection with geometrical properties and might, very likely, open up this subject to re-interpretation. The main scope of the paper is not to provide a way to exploit the new symmetries directly into the dynamic equation, but rather to provide a method to decide whether a certain system of coordinates has the property (2). The feature of separation of the kinetic energy of the center of mass is an essential prerequisite to all formulations of dynamic theories of the N-body problem (Lagrangian mechanics, Hamiltonian mechanics, quantum mechanics, etc).

2. Derivation of the main result

In medias res, let us consider coordinate transformations of the type

$$\vec{x}' = A\vec{x} \tag{3}$$

where the components of the vectors $\vec{x}, \vec{x}'$ are connected to each other by

$$x_i' = \sum_{j=1}^{n} a_{ij} x_j. \tag{4}$$

It is convenient to remember that each of these components might also represent a multidimensional vector.

The relations holding among the corresponding partial derivatives are

$$\frac{\partial}{\partial x_k} = \sum_{i=1}^{n} \frac{\partial x_i'}{\partial x_k} \frac{\partial}{\partial x_i'} = \sum_{i=1}^{n} a_{ik} \frac{\partial}{\partial x_i'} \tag{5}$$

where we have used

$$\frac{\partial x_i'}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{j=1}^{n} a_{ij} x_j = \sum_{j=1}^{n} a_{ij} \delta_{jk} = a_{ik}. \tag{6}$$

We are looking for the conditions to impose on the generic coordinate transformation that bring the sum of pure second derivatives of the unprimed coordinates into the sum of pure second derivatives of the primed coordinates without introducing mixed derivatives. In other words, for each $k = 1, \ldots, n$, if

$$\frac{\partial^2}{\partial x_k^2} = \left(\sum_{i=1}^{n} a_{ik} \frac{\partial}{\partial x_i'} \right) \left(\sum_{j=1}^{n} a_{jk} \frac{\partial}{\partial x_j'} \right) = \sum_{i,j=1}^{n} a_{ik} a_{jk} \frac{\partial^2}{\partial x_i' \partial x_j'} \tag{7}$$

is the transformation of the second derivatives, the $n(n-1)/2$ conditions to forbid the presence of mixed derivatives are

$$\sum_{k=1}^{n} a_{ik}a_{jk} = 0 \quad \forall\{i,j\}/i \neq j = \{1,\ldots,n\}. \tag{8}$$

These $n(n-1)/2$ equations form a system with n^2 unknowns; hence $n(n+1)/2$ matrix elements might arbitrarily be chosen. In order to ensure that the last of the coordinates always coincides with the position of the center of mass, the elements in the last row must take the form $a_{ni} = 1/n, \forall i = 1,\ldots,n$, and hence upon simplification the system (8) is replaced by

$$\begin{cases} \left\{ \sum_{k=1}^{n} a_{ik}a_{jk} = 0 \quad \forall\{i,j\}/i \neq j = \{1,\ldots,n-1\} \right. \\ \left\{ \sum_{k=1}^{n} a_{ik} = 0 \qquad i = \{1,\ldots,n-1\} \right. \end{cases} \tag{9}$$

where the first line represents a subsystem of $(n-2)(n-1)/2$ conditions of the form (8) with indexes i, j restricted to avoid n and the second line represents $n-1$ simpler conditions. In general the system (9) has $n^2 - n$ unknowns, of which $(n-1)(n-2)/2$ and $(n-1)$ are set and the remaining matrix elements can be chosen arbitrarily. Therefore, there are entire classes of transformations that comply with the requirement (2). Oftentimes it is convenient to impose that at least some of the vectors correspond to relative position vectors and this implies transformation matrices with (in some rows) only two elements different from 0 and equal to 1 and -1, respectively.

3. Case of two particles

As an introductory example we discuss the case of two particles, $n = 2$. One has the matrix

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}. \tag{10}$$

Condition (8) takes (twice) the form $a_{11}a_{21} + a_{12}a_{22} = 0$ that, bearing in mind that we wish to keep $a_{21} = a_{22} = 1/2$, has only one solution $a_{12} = -a_{11}$.

Leaving aside the trivial $a_{11} = a_{12} = 0$, that is unacceptable to our scope, we have the freedom to choose the value of one of the matrix elements. Note that with $a_{11} = 1$ it is exactly the coordinate transformation that takes the position of two particles into the relative coordinate plus the coordinate of the center of mass, depicted in figure 1. Any other choice would have simply altered the modulus or sign of the internal coordinate $\vec{x}_1'$ without changing its direction.

The most general matrix we can use for two particles is

$$A_2(a) = \begin{pmatrix} a & -a \\ 1/2 & 1/2 \end{pmatrix} \tag{11}$$

with freedom on a. The transformation of coordinates of figure 1 corresponds to $A_2(1)$. Note that these matrices form an additive group under the law of composition obtained by the operation of standard matrix addition and subsequent division by 2. Although there is nothing exceptionally new about this composition law (it is essentially matrix addition), I will indicate it with the $\dotplus$ symbol, for the sake of brevity. Instead these matrices are *not* a group under usual matrix multiplication. In other words, we do not try to apply $A_2(b)$ to $A_2(a)$ and then to the column vector $(\vec{x}_1, \vec{x}_2)$: by doing so one ends up with something completely

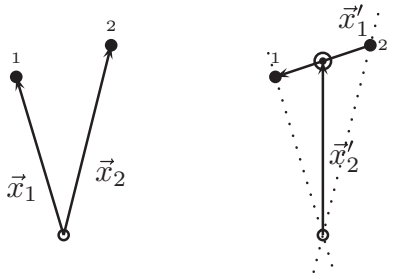

Figure 1. Transformation discussed in the text for two particles (black dots). Hollow circles represent the external reference point and double circle represents the particles' center of mass. Dotted lines are rails (see the text).

useless. But we rather apply the composition $A_2(a) \dot{+} A_2(b)$ to the column vector: this will give a transformation of the same type again. The meaning of this group is that all the infinite possible transformations that preserve the pure second derivatives and separate the second derivative with respect to the center of mass coordinate are essentially equivalent, and therefore the parameter a can be set to 1 without loss of information. The entire class can be seen geometrically as follows: in figure 1 draw the two lines connecting the external reference point with 1 and 2 and call them rails; shift the vector $\vec{x}'_1$ along the rails, keeping it parallel to the original and adjusting the length in order to maintain its extremes on their rails. The infinite set of vectors that are obtained by this parallel expansion/contraction procedure maps one-to-one to the real numbers a.

4. Case of three particles

In the case of three particles, $n = 3$, the matrix is

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \tag{12}$$

and the conditions are

$$\begin{cases} a_{11}a_{21} + a_{12}a_{22} + a_{13}a_{23} = 0 \\ a_{11}a_{31} + a_{12}a_{32} + a_{13}a_{33} = 0 \\ a_{21}a_{31} + a_{22}a_{32} + a_{23}a_{33} = 0 \end{cases} \tag{13}$$

that with $a_{31} = a_{32} = a_{33} = 1/3$ can be simplified to a system of three equations with six unknowns

$$\begin{cases} a_{11}a_{21} + a_{12}a_{22} + a_{13}a_{23} = 0 \\ a_{11} + a_{12} + a_{13} = 0 \\ a_{21} + a_{22} + a_{23} = 0 \end{cases} \tag{14}$$

where two of the three equations have the form suggested in (9). Therefore, one has the freedom to choose three elements and deduce the others according to (14).

Using, for instance, $a_{11} = 1$, $a_{12} = -1$ and $a_{22} = 1/2$ one gets for $\vec{x}'$ a possible set of Jacobi coordinates containing the position of the total center of mass, the relative coordinate between particles 1 and 2 and the relative coordinate between particle 3 and the minor center of mass of particles 1 and 2, as shown in figure 2.

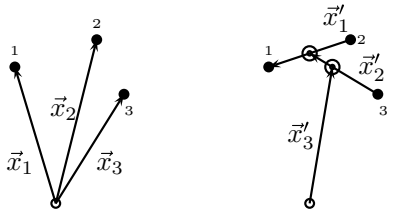

Figure 2. Transformation discussed in the text for three particles (black dots). Hollow circles represent the external reference point and double circles represent the particles' total and partial centers of mass.

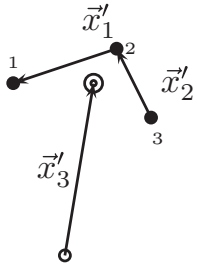

Figure 3. A coordinate system that does not obey the set of equations (14) and thus does not allow for the separation of the center of mass kinetic energy.

The set of equations (14) is important, because at a glance it shows that, for example, certain coordinates systems do not have the right property of the separation of the center of mass. Consider the coordinates as shown in figure 3, sometimes called necklace or sequential coordinates[1]. Using $a_{11} = 1$, $a_{12} = -1$ one gets $a_{13} = 0$, $a_{21} = a_{22}$ and therefore $2a_{22} + a_{23} = 0$. While the choice of the preceding example works well, the choice $a_{22} = 1$ and $a_{23} = -1$ *does not satisfy this last equation and therefore does not permit the separation of the center of mass* as described by (2).

To underline the importance of the present discussion let me add that the system of coordinates shown in figure 3, that appears very natural, has been ruthlessly employed without caring for the separation of the center of mass motion, thus leading to incorrect results! The coordinate system of figure 2 must be preferred, as well as any other system that obeys conditions (14).

The most general matrix for three particles is

$$A_3(a,b,c) = \begin{pmatrix} a & b & -a-b \\ c & -c\dfrac{2a+b}{a+2b} & c\dfrac{a-b}{a+2b} \\ 1/3 & 1/3 & 1/3 \end{pmatrix} \tag{15}$$

with arbitrary a, b, c. These matrices are not in general a group as before, but remarkably they can still form an additive group under the operation $\dotplus$ by restricting some of the parameters. This can be accomplished only in two ways: either $b = ka$ or $a = k'c - 2b$, where k and

[1] A folklore note: it is precisely the fact that I was considering the necklace coordinates in connection with many-body nuclear physics models that brought my attention to the fact that this problem was not thoroughly known and to the formulation of the general conditions under which the separation is possible.

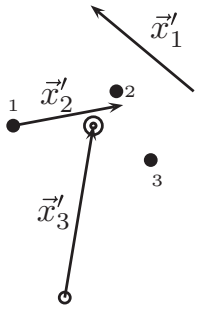

Figure 4. A rather unusual coordinate system corresponding to $A_3(1/2, 1, -1)$ that nevertheless allows for the separation of the center of mass kinetic energy.

k' are constants. By imposing these two conditions the resulting transformation matrices are respectively

$$A_3^{(1)}(a, c)_k = \begin{pmatrix} a & ka & -a(1+k) \\ c & -c\dfrac{2+k}{1+2k} & c\dfrac{1-k}{1+2k} \\ 1/3 & 1/3 & 1/3 \end{pmatrix} \tag{16}$$

$$A_3^{(2)}(b, c)_{k'} = \begin{pmatrix} k'c - 2b & b & b - k'c \\ c & -2c + \dfrac{3b}{k'} & c - \dfrac{3b}{k'} \\ 1/3 & 1/3 & 1/3 \end{pmatrix} \tag{17}$$

where the superscripts in parenthesis just denote an arbitrary labeling. The difference between these two matrix groups lies in the fact that one has two arbitrary parameters in the same column, and the other in different columns and, upon reshuffling of the columns, these are the only two possible ways. It can be noted that the transformation to Jacobi coordinates of figure 2 is an element of both groups that corresponds to

$$A_3(1, -1, 1/2) = A_3^{(1)}(1, 1/2)_{-1} = A_3^{(2)}(-1, 1/2)_{-2}. \tag{18}$$

An alternative set of Jacobi coordinates is given by $A_3(0, 1, -1)$. Notably this is not an element of $A_3^{(1)}$, but it is an element of $A_3^{(2)}(1, -1)_{-2}$. However, by noting that its matrix corresponds to the previous Jacobi coordinates matrix upon reordering of the columns, one can see that this fact is simply explained by the arbitrariness in choosing the free matrix elements in (15): we have filled the upper-left triangle with arbitrary parameters and determined the rest, but one could have made other choices as well. Summarizing, one must keep in mind that there are two levels of arbitrariness in the procedure of calculation of the matrices: (i) it is arbitrary to choose which elements are parameters and which are functions of these parameters and, (ii) the values of the parameters themselves are arbitrary.

Several choices of parameters a, b, c can be traced back to a 'rail projection' of a set of Jacobi coordinates, as, for instance, $A_3(1, 1, 1)$: the first coordinate coincides with $\vec{x}'_1$ of figure 2, the third is the center of mass coordinate $\vec{x}'_3$ as in all other cases, but the second is just an expansion of $\vec{x}'_2$ of figure 2 along the two rails connecting the reference point with 3 and with the center of mass of particles 1 and 2. This is analogous to the case already discussed for two particles. Apart from these cases, there are others that, despite their strange look, are equally good at separating out exactly the kinetic energy of the center of mass. Take for example $A_3(1/2, 1, -1)$ that gives the coordinate system depicted in figure 4. Albeit

this might be useless to the solution of the many-body problem, it is a viable alternative to Jacobi coordinates. This example shows clearly that, when $n > 2$, the group structure has a geometrical interpretation that is wider than the parallel expansion/contraction along the rails described above, but several subsets of all possible transformations still have this interpretation. In particular for matrix (16), it is possible to find fixed rails, because a and c amount to a multiplicative constant for $\vec{x}_1'$ and $\vec{x}_2'$ respectively, but in this case, by changing k, one is not only shifting the vector's tips along the rails, but also changing its direction accordingly. The interpretation of (17) is instead less obvious, because two parameters enter at the same time into several matrix elements.

5. General case

For n particles we return to the system (9). The corresponding transformation matrix that maps the initial set of coordinates into a set of coordinates that allows the exact separation of the center of mass kinetic energy can be schematically divided in the following way:

$$A_n(a_1, \ldots, a_p) = \begin{pmatrix} a & \cdots & c_2 \\ \vdots & \iddots & \vdots \\ & \cdots\ c_1 & \\ 1/n & \cdots & \end{pmatrix} \tag{19}$$

where the n matrix elements of the last row are all equal to $1/n$. Conditions (9.2) are used to determine, for example, the remaining $n-1$ elements of the last column (one could have equivalently chosen another column):

$$a_{in} = -\sum_{k=1}^{n-1} a_{ik} \qquad i = \{1, \ldots, n-1\}. \tag{20}$$

Conditions (9) are used to set the $(n-1)(n-2)/2$ matrix elements of the lower triangle as functions of the arbitrary $p = n(n-1)/2$ matrix elements of the upper triangle, starting from the pair $\{i, j\} = \{1, 2\}$ and proceeding row by row. Matrices (19) most certainly do not form a group under $\dotplus$, but it is still possible that, as in the case $n = 3$, they would do so by restricting the number of parameters under certain special conditions.

6. Illustrative examples

Let us give an example of the usefulness of conditions (9). With reference to figure 5, suppose that we wish to use the internal coordinates of the two subsystems formed by particles 1–2 and 3–4 and, in addition, we also want the right property of separating the total kinetic energy center of mass (into the new coordinate $\vec{x}_4'$).

By filling up the transformation matrix for four particles with the proper values for the first, third and fourth rows, we get

$$\begin{pmatrix} 0 & 0 & 1 & -1 \\ a & a & -a & -a \\ 1 & -1 & 0 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 \end{pmatrix}. \tag{21}$$

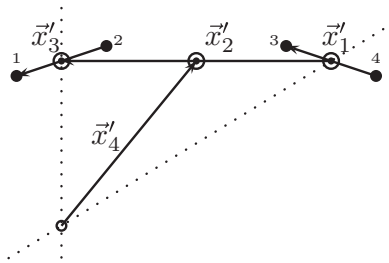

Figure 5. Coordinate system corresponding to $A_4(0, 0, 1, 1/2, 1/2, 1)$. The rails are indicated as dotted lines. This system can be used to model scattering of two deuterons for example.

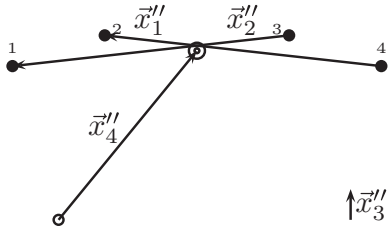

Figure 6. Coordinate system corresponding to $A_4(0, 1, 0, 1, 0, 1)$. This system clearly has the property (2), but it would have been difficult to guess, without recurring to the transformation matrix.

Therefore, the entire class of possible transformations in this particular case reduces to all the vectors with a direction parallel to that of the center of mass of 3–4 to the center of mass of 1–2, or, in other words all expansions/contractions along the rails shown in figure 5 as dotted lines. With the choice $a = 1/2$ we have the simplest of these vectors, i.e. $\vec{x}'_2$ of figure 5. These coordinates are suitable to describe, for instance, the scattering of two deuterons, where the total wavefunction can be expanded in terms of products like $\phi_{12}(\vec{x}'_3)\phi_{34}(\vec{x}'_1)\psi(\vec{x}'_2)$, where ϕ are internal wavefunctions that separately describe the subsystems 1–2 and 3–4 and ψ is the relative motion wavefunction between the two subsystems.

Note that only vectors that have their extremes on the rails are acceptable; any other choice would not separate the center of mass motion correctly. Although the vector $\vec{x}'_2$ of figure 5 could have been guessed, other correct choices would have been more difficult to predict without the above matrix. For example, one could have been tempted by the coordinate system formed by vectors that connect particles 1 and 2, particles 2 and 3 and finally particles 3 and 4 (together with the vector $\vec{x}'_4$ of figure 5): this choice does not work and this can be seen at a glance by looking at the proper matrix. On the other hand, a system of coordinates that one would not even take into consideration are seen to possess the separation property. Let us consider, for instance, the coordinate system proposed in figure 6. It is very difficult to guess that it is a good one, based only on first principles, but upon inspection of the corresponding transformation matrix it clearly satisfies the conditions on the mixed derivatives. In particular, the vector $\vec{x}''_3$ is the difference between vectors $\vec{x}'_1$ and $\vec{x}'_3$ of the preceding figure.

Several other systems might be treated with coordinates of this type: cluster states in light nuclei, tetratomic molecules and so on.

7. Conclusions

In conclusion, this paper discusses the most general conditions to impose on transformations of coordinates that allow for the exact separation of the total center of mass kinetic energy, obtaining a set of equations (8). These equations show that there are classes of coordinates systems that can be used in place of the usual Jacobi coordinates, achieving the same goal of the elimination of the center of mass energy. The application to small numbers of particles has been discussed and it is found that a curious additive group structure is hidden in these transformation matrices. The analysis reveals a connection with a simple geometrical interpretation. I believe that these results can be of some importance to quantum many-body models based on the solution of the non-relativistic Schrödinger equation and that the new group structure might reveal further hidden symmetries and analogies that might help to advance this field. Although it is difficult to envision how this more general separation of the center of mass motion might help to simplify the dynamic equations, it is nevertheless a common prerequisite to many important theories of the *N*-body problem.

References

[1] Fano U, Green D, Bohn J L and Heim T A 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** R1–37
[2] Meremianin A V and Briggs J S 2003 *Phys. Rep.* **384** 121–95
[3] Greiner W 2001 *Quantum Mechanics, An Introduction* 4th edn (Berlin: Springer)
[4] Smith F T 1960 *Phys. Rev.* **120** 1058