Fractional Cassini Coordinates

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1. Introduction

For a given problem an appropriate choice of a specific coordinate system may indeed simplify calculations significantly. Special coordinate systems are often used to solve various problems in different areas of e.g. mathematics, natural sciences or engineering. As part of the classical canon of standard tools they are well documented.

A typical example is the use of spherical coordinates for isotropic problems or in classical mechanics the use of cylinder coordinates to determine the moment of inertia with respect to a given rotational axis. Within atomic physics, in a series of seminal papers Hylleraas used prolate elliptic coordinates to calculate the eigenfunctions and values of the two electron Schrödinger equation for the helium-atom, applying the Ritz variational principle.

While elliptical coordinates are very efficient in atomic physics for two-center problems for rather small center distances, they become less efficient with increasing...
distance between ions\[5\]. For such cases, Cassini-coordinates\[6\] are the better choice, which are defined as:

\[
w = \sqrt{r_1 r_2} \quad \text{(1)}
\]

\[
\theta = \frac{1}{2}(\tau_1 + \tau_2) \quad \text{(2)}
\]

The classical example is the solution of the two-center Dirac-equation for the study of spectra of quasi-molecules\[7\], which are formed during slow heavy-ion collisions\[4,8\], since the corresponding potential \(V\) is the superposition of two electron-nucleus potentials, see figure\[11\]. In this case, \(r_i\) is the distance between the electron and the \(i\)-th nucleus, and \(\tau_i\) is the angle between the inter nuclear axis and the vector \(\vec{r}_i\).

In nuclear physics, asymmetric nuclear shapes for large deformation have been calculated using symmetric Cassini ovaloids, where the asymmetry was expanded in a series of Legendre polynomials\[9,10\]. Since symmetric Cassini-coordinates are well suited for symmetric problems, it is tempting and straightforward to extend the definition of the symmetric Cassini coordinate system to a larger family of asymmetric orthogonal fractional coordinate systems in order to describe asymmetric...
problems appropriately.

2. Properties of fractional Cassini coordinates

For reasons of simplicity, we first restrict our presentation of a non symmetric fractional extension of the Cassini-coordinates to \( \mathbb{R}^2 \) and in a second step extend the result to rotationally symmetric coordinates in \( \mathbb{R}^3 \).

Let us assume a collection of \( n \) focal points \( F \) in the x-y-plane with coordinates \( \{ x_i, y_i \} \) and a corresponding set of fractional exponents \( \{ \alpha_i \} \in \mathbb{R} \). We define a new pair of coordinates \( x^\mu = \{ w(x, y), \theta(x, y) \} \):

\[
w^{\alpha_s} = \prod_{i=1}^{n} r_i^{\alpha_i}, \quad \theta = \sum_{i=1}^{n} \alpha_i \arctan \left( \frac{y - y_i}{x - x_i} \right)
\]

with

\[
\alpha_s = \sum_{i=1}^{n} \alpha_i, \quad r_i = \sqrt{(x - x_i)^2 + (y - y_i)^2}
\]

which extend the standard symmetric Cassini coordinate set (1), (2) to the fractional case.

The transformation properties of the \( g_{\mu\nu} \) tensor are given as

\[
g_{\mu\nu} = \frac{\partial x^i}{\partial x^\mu} \frac{\partial x^j}{\partial x^\nu} g_{ij}
\]

In order to derive the factors \( \frac{\partial x^i}{\partial x^\mu} \), we apply the derivative operators \( \partial_\mu \) transformation equations (3) and (4) and obtain

\[
(w^{\alpha_s})|_{\mu} = w^{\alpha_s} \left\{ \left( \sum_{i=1}^{n} \alpha_i \frac{x - x_i}{r_i^2} \right) x|_\mu + \left( \sum_{i=1}^{n} \alpha_i \frac{y - y_i}{r_i^2} \right) y|_\mu \right\}
\]

\[
(\alpha_s \theta)|_{\mu} = \left\{ -\left( \sum_{i=1}^{n} \alpha_i \frac{y - y_i}{r_i^2} \right) x|_\mu + \left( \sum_{i=1}^{n} \alpha_i \frac{x - x_i}{r_i^2} \right) y|_\mu \right\}
\]

This is a linear system of equations to determine \( x|_\mu \).

With the abbreviations

\[
\bar{x} = \sum_{i=1}^{n} \alpha_i \frac{x - x_i}{r_i^2}, \quad \bar{y} = \sum_{i=1}^{n} \alpha_i \frac{y - y_i}{r_i^2}
\]
we obtain in matrix form:

\[
\begin{pmatrix}
w^{\alpha_s} \bar{x} & w^{\alpha_s} \bar{y} \\
-\bar{y} & \bar{x}
\end{pmatrix}
\begin{pmatrix}
x|_w \\
y|_w
\end{pmatrix} = \begin{pmatrix}
\alpha_s w^{\alpha_s - 1} \\
0
\end{pmatrix}
\] (12)

\[
\begin{pmatrix}
w^{\alpha_s} \bar{x} & w^{\alpha_s} \bar{y} \\
-\bar{y} & \bar{x}
\end{pmatrix}
\begin{pmatrix}
x|_\theta \\
y|_\theta
\end{pmatrix} = \begin{pmatrix}
0 \\
\alpha_s
\end{pmatrix}
\] (13)

for the derivatives follows:

\[
\frac{\partial x}{\partial w} = \frac{\alpha_s \bar{x}}{w(\bar{x}^2 + \bar{y}^2)}
\] (14)

\[
\frac{\partial y}{\partial w} = \frac{\alpha_s \bar{y}}{w(\bar{x}^2 + \bar{y}^2)}
\] (15)

\[
\frac{\partial x}{\partial \theta} = -\frac{\alpha_s \bar{y}}{\bar{x}^2 + \bar{y}^2}
\] (16)

\[
\frac{\partial y}{\partial \theta} = \frac{\alpha_s \bar{x}}{\bar{x}^2 + \bar{y}^2}
\] (17)

and finally for the \(g^{fC}_{\mu\nu}\) tensor for the fractional Cassini coordinates:

\[
g^{fC}_{\mu\nu} = \begin{pmatrix}
\frac{\alpha_s^2}{w^2} & \frac{1}{w^2 (\bar{x}^2 + \bar{y}^2)} \\
0 & \frac{\alpha_s^2}{w^2} \\
\frac{1}{w^2 (\bar{x}^2 + \bar{y}^2)} & 0
\end{pmatrix}
\] (18)

Since the \(g_{\mu\nu}\) tensor is diagonal, the coordinate transformation is orthogonal.

In figures (2)-(4) we compare the orthogonal meshes of constant \(\{w, \theta\}\) (which in nuclear physics may serve as a description of corresponding shapes for a nucleus undergoing a binary or ternary fission process) to corresponding Coulomb potential \(V_c\) for point charges

\[
V_c = -\sum_{i=1}^{n} \frac{Z_i}{r_i}
\] (19)

for asymmetric two center, mirror symmetric and asymmetric three center configurations. With appropriately chosen values for the powers \(\{\alpha_i\}\) the fractional Cassini-coordinates may be adjusted to follow the equi-potential lines surprisingly well.

3. Special cases

The following special cases with \(\{\alpha_i = 1\}\) are included in the definition:

- One focal point \(n = 1\)
Polar coordinates with \(F_1 = \{0, 0\}\)

\[
g_{\mu\nu}^{pol} = \begin{pmatrix}
1 & 0 \\
0 & w^2
\end{pmatrix}
\] (20)
Fig. 2. Contours of the orthogonal asymmetric fractional Cassini-coordinate system for two focal points \( F_1 = \{-2, 0\} \), \( F_2 = \{+2, 0\} \) and \( (\alpha_1 = 0.5, \alpha_2 = 0.92) \). Solid thick lines show \( w = \text{const} \), thin lines show \( \theta = \text{const} \). Bold line at \( y = 0 \) indicates the branch cut for \( \theta = \{0, 2\pi\} \). Dashed lines show the corresponding two center Coulomb potential with \( Z_1 = 50 \) and \( Z_2 = 92 \).

Transformation equations (3) and (4) simply result as:

\[
\begin{align*}
    w &= \sqrt{x^2 + y^2} \\
    \theta &= \arctan\left(\frac{y}{x}\right)
\end{align*}
\]  (21)

\[
\begin{align*}
    \theta &= \frac{1}{2}(\arctan\left(\frac{y}{x+c}\right) + \arctan\left(\frac{y}{x-c}\right))
\end{align*}
\]  (22)

- Two focal points \( n = 2 \)

  Cassini coordinates with \( F_1 = \{-c, 0\} \) and \( F_2 = \{c, 0\} \)

\[
\begin{align*}
    g_{\mu\nu} &= \begin{pmatrix}
        \frac{w^2}{x^2+y^2} & 0 \\
        0 & \frac{w^4}{x^2+y^2}
    \end{pmatrix}
\end{align*}
\]  (23)

Transformation equations (3) and (4) follow as:

\[
\begin{align*}
    w^2 &= r_1 r_2 \\
    \theta &= \frac{1}{2}(\arctan\left(\frac{y}{x+c}\right) + \arctan\left(\frac{y}{x-c}\right))
\end{align*}
\]  (24)

with

\[
\begin{align*}
    r_1 &= \sqrt{(x + c)^2 + y^2} \\
    r_2 &= \sqrt{(x - c)^2 + y^2}
\end{align*}
\]  (25)
Fig. 3. Contours of the orthogonal mirror symmetric fractional Cassini-coordinate system for three focal points \((F_1 = \{-2, 0\}, F_2 = \{0, 0\}, F_3 = \{2, 0\})\) and \((\alpha_1 = 3, \alpha_2 = 4, \alpha_3 = 3)\). Solid thick lines show \(w = \text{const}\), thin lines show \(\theta = \text{const}\). Bold line at \(y = 0\) indicates the branch cut for \(\theta = \{0, 2\pi\}\). Dashed lines show the corresponding three center Coulomb potential with \(Z_1 = 40, Z_2 = 82\) and \(Z_3 = 40\).

Using the identity (4.4.36) from\(^{11}\)

\[
\arctan(u) + \arctan(v) = \arctan\left(\frac{u + v}{1 - uv}\right)
\]

we obtain

\[
w^4 = (x^2 + y^2)^2 - 2c^2(x^2 - y^2) + c^4
\]

\[
\theta = \frac{1}{2} \arctan\left(\frac{2xy}{x^2 - y^2 - c^2}\right)
\]

Now we will determine the term \(x^2 + y^2\) in the \(g_{\mu\nu}\) tensor as a function of \(x^\mu\). In order to simplify procedure we introduce the variables \(P\) und \(Q\):

\[
P = x^2 + y^2
\]

\[
Q = x^2 - y^2
\]

Inserting in (28) and (30):

\[
w^4 = P^2 - 2c^2Q + c^4
\]

\[
\theta = \frac{1}{2} \arctan\left(\frac{\sqrt{P + Q}\sqrt{P - Q}}{Q - c^2}\right)
\]
Fig. 4. Contours of the orthogonal asymmetric fractional Cassini-coordinate system for three focal points \( F_1 = \{-2, 0\}, F_2 = \{0, 0\}, F_3 = \{2, 0\} \) and \( \alpha_1 = 0.2, \alpha_2 = 0.28, \alpha_3 = 0.5 \). Solid thick lines show \( w = \text{const} \), thin lines show \( \theta = \text{const} \). Bold line at \( y = 0 \) indicates the branch cut for \( \theta = \{0, 2\pi\} \). Dashed lines show the corresponding three center Coulomb potential with \( Z_1 = 20, Z_2 = 28 \) and \( Z_3 = 50 \).

or

\[
w^4 = P^2 - Q^2 + (Q - c^2)^2 \tag{35}
\]

\[
\tan^2(2\theta) = \frac{P^2 - Q^2}{(Q - c^2)^2} \tag{36}
\]

Explicitly we obtain for \( Q \):

\[
Q = c^2 \pm \frac{w^2}{\sqrt{1 + \tan^2(2\theta)}} \tag{37}
\]

and \( P \):

\[
P = \sqrt{w^4 + c^4 \pm \frac{2c^2w^2}{\sqrt{1 + \tan^2(2\theta)}}} \tag{38}
\]

with (4.3.25) and (4.3.26) from\[\text{[1]}\]

\[
\frac{1}{\sqrt{1 + \tan^2(2\theta)}} = \cos(2\theta) \tag{39}
\]

\[
= \cos^2(\theta) - \sin^2(\theta) \tag{40}
\]
We finally obtain the $g_{\mu\nu}$ for Cassini coordinates in the standard, familiar form:

$$g_{\mu\nu} = \frac{w^2}{\sqrt{w^4 + c^4 + 2c^2w^2\cos(2\theta)}} \begin{pmatrix} 1 & 0 \\ 0 & w^2 \end{pmatrix}$$

(42)

4. Extension to cylindrically symmetric coordinate systems

Since the explicit form of an orthogonal fractional extension of the Cassini coordinates in two dimensions has been derived, we finally propose a transition from $R^2$ (with $g^{(2)}_{\mu\nu}$) to $R^3$ (with $g^{(3)}_{\mu\nu}$), to obtain cylindrically symmetric fractional coordinate systems, which are best suited to describe e.g. cylindrically symmetric two center potentials in atomic physics and asymmetric nuclear shapes in nuclear fission processes, respectively.

Let us recall, that a coordinate transformation in $R^2$ from Cartesian to polar coordinates, given by

$$x = f(r, \theta)$$

$$y = g(r, \theta)$$

determines the corresponding two dimensional $g^{(2)}_{\mu\nu}$ tensor:

$$g^{(2)}_{rr} = \left(\frac{\partial f}{\partial r}\right)^2 + \left(\frac{\partial g}{\partial r}\right)^2$$

(45)

$$g^{(2)}_{r\theta} = \frac{\partial f}{\partial r} \frac{\partial f}{\partial \theta} + \frac{\partial g}{\partial r} \frac{\partial g}{\partial \theta}$$

(46)

$$g^{(2)}_{\theta\theta} = \left(\frac{\partial f}{\partial \theta}\right)^2 + \left(\frac{\partial g}{\partial \theta}\right)^2$$

(47)

Rotating this coordinate system around the $x$-axis and introducing cylinder coordinates in $R^3 \{\rho, z, \phi\}$, we apply a mapping of the above derived $g^{(2)}_{\mu\nu}$ with two dimensional polar coordinates, where the metric tensor $g^{pol}_{\mu\nu}$ is given by (20):

$$g^{pol}_{\mu\nu} = \begin{pmatrix} 1 & 0 \\ 0 & \rho^2 \end{pmatrix}$$

(48)

The transition follows formally by the replacements:

$$x \rightarrow z$$

(49)

$$y \rightarrow \rho$$

(50)

It follows

$$z = f(r, \theta)$$

(51)

$$\rho = g(r, \theta)$$

(52)
and

\[
\frac{\partial z}{\partial \phi} = 0 \\
\frac{\partial \rho}{\partial \phi} = 0
\]  

(53)

(54)

This yields the \( g_{\mu\nu} \) tensor using the new coordinate set

\[
g^{(3)}_{\mu\nu} = \begin{pmatrix}
g^{(2)}_{11} & g^{(2)}_{12} & 0 \\
g^{(2)}_{21} & g^{(2)}_{22} & 0 \\
0 & 0 & \rho^2
\end{pmatrix}
\]  

(55)

The explicit form of \( g^{(3)}_{33} \) follows from (52) and (44).

Insertion to (55) yields the general result for an arbitrarily given \( g^{(2)}_{\mu\nu} \):

\[
g^{(3)}_{\mu\nu} = \begin{pmatrix}
g^{(2)}_{11} & g^{(2)}_{12} & 0 \\
g^{(2)}_{21} & g^{(2)}_{22} & 0 \\
0 & 0 & g^2(r, \theta)
\end{pmatrix}
\]  

(56)

Hence we derived a direct method to transform any two dimensional coordinate system with given \( g^{(2)}_{\mu\nu} \) to a three dimensional cylindrically symmetric coordinate system with \( g^{(3)}_{\mu\nu} \).

According to (18) off-diagonal elements of the \( g^{(2)}_{\mu\nu} \) tensor for the fractional Cassini-coordinates are vanishing, therefore we obtain finally for asymmetric fractional Cassini-coordinates:

\[
g^{fC}_{\mu\nu} = \begin{pmatrix}
g^{fC}_{11} & 0 & 0 \\
0 & g^{fC}_{22} & 0 \\
0 & 0 & g^2(r, \theta)
\end{pmatrix}
\]  

(57)

5. Conclusion

We have derived a new family of orthogonal coordinate systems, which extend the symmetric Cassini coordinates in a reasonable way to the fractional case, introducing a set of fractional exponential coefficients \( \{\alpha_i\} \in \mathbb{R} \). In addition we have derived a general procedure to extend orthogonal coordinate systems from \( \mathbb{R}^2 \) to the cylindrically symmetric case in \( \mathbb{R}^3 \).

This new set of asymmetric, fractional coordinate systems may reduce the effort to solve asymmetric two (and more)-center problems in all branches of physics.

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