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CALCULATION OF ORBITAL AND SPIN LIE OPERATORS

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In this report the problems of orbital and spin nonlinear calculations are discussed. The introduction of the special $\mathcal{P}$- and $\mathcal{D}$-functions allows us to formalize the determination of the orbital and spin Lie operators and to apply the systems of the analytical calculations to find them. An increase in the accuracy of numerical calculations can be achieved through the usage of these functions instead of the standard math-library functions cos, sin and etc.

KEY WORDS: Spin motion, Lie algebra, Lie operators

1 INTRODUCTION

The problem of the nonlinear orbital and spin dynamics can be considered as one of the most urgent ones. The reasons are as follows. Firstly, the magnetic structure of the modern accelerators has become more rigid and therefore, nonlinear effects have turned to be more significant. Secondly, unfortunately there is as yet no universal method for these tasks.

Different approaches are used in accelerator physics. The choice between them depends on the problem or on the author's preferences. We have used Lie technique but the subject matter of this report can be applied to any other approach.

In our case it is necessary to find the map from initial orbital and spin vectors to its final values. The orbital and spin Lie operators determine this map.[1,2]

Special rules exist for, Lie operators calculations. But in practice, rules are usually very complicated, which makes the calculations too cumbersome. The usage of computing systems in analytical calculations should be considered as a good solution.

The rules of Lie operators determination include repeated integrations of different polynomials of the trigonometrical functions. As a result of these integrations the constructions, which are a division of small differences by other small differences, appear. For this reason the accuracy of the numerical calculations decreases. Both of these problems can be solved by the introduction of the special $\mathcal{P}$- and $\mathcal{D}$-functions. The rules for the operations with these functions allow us to formalize the calculations and to apply systems of analytical calculations for of Lie operators determination. An increase in the accuracy of numerical calculations is achieved through the usage of explicit expansion $\mathcal{P}$- and $\mathcal{D}$-functions in the series. These series converge very quickly in the cases of accelerator problems since the function's arguments are less than unit usually.

The plan of the paper is as follows. In parts 2 and 3 special $\mathcal{P}$- and $\mathcal{D}$-functions are discussed. They are offered in order to obtain explicit expressions for the orbital and spin Lie operators for all types of collider elements. The application of the analytical calculations system (REDUCE) to compute these expressions is considered in the following part. Orbital and spin matrices and Lie operator formulae for different elements of the collider were calculated by code HAMIL.RED and few of them are presented in the last part. The results for orbital motion in the case of the homogeneous field can be compared with.[3] These examples show advantages of usage of $\mathcal{P}$- and $\mathcal{D}$-functions for simple as well as complicated expressions.

Lie operators, which were obtained by computer code HAMIL.RED, were programed in FORTRAN code SPINLIE for calculations of polarization in colliders.[2,4,5]

2 $\mathcal{P}$-FUNCTIONS

For practical calculation of the Lie operators it is useful to introduce special $\mathcal{P}$-functions. Expressions for them include, as a rule, complicated combinations of trigonometrical functions, since the usage of $\mathcal{P}$-functions (and $\mathcal{D}$-functions; see the next part) allows us to formalize calculations and to use them for computer analytical system.

Let us introduce the function $\mathcal{P}_i(Q, s)$ as a "single" series

$$\mathcal{P}_i(Q, s) = s^i \sum_{j=0}^{\infty} \frac{(-Q^2 s^2)^j}{(2j+i)!}.$$

It is easy to verify that the relations between the functions $\mathcal{P}_i(Q, s)$ and usual trigonometrical ones are determined by the following expressions:

$$\mathcal{P}_0(Q, s) = \cos Qs,$$

$$\mathcal{P}_1(Q, s) = \frac{\sin Qs}{Q} = s\left(\frac{\sin Qs}{Qs}\right),$$

$$\mathcal{P}_2(Q, s) = \frac{1 - \cos Qs}{Q^2} = s^2\left(\frac{1 - \cos Qs}{(Qs)^2}\right),$$

$$\mathcal{P}_3(Q, s) = \frac{s - \frac{\sin Qs}{Q}}{Q^2} = s^3\left(\frac{1 - \frac{\sin Qs}{Qs}}{(Qs)^2}\right)$$

and etc. The usage of $\mathcal{P}$-functions allows us to eliminate small denominators (Q and it powers) in the right parts of these expressions.

$\mathcal{P}$-functions have the following properties:

$$\mathcal{P}_i(0, s) = \frac{s^i}{i!},$$

$$\mathcal{P}_i(Q, 0) = \begin{cases} 0 & \text{if } i \neq 0, \\ 1 & \text{if } i = 0 \end{cases}$$

The following recurrent expressions are valid:

$$\mathcal{P}_{i+2}(Q, s) = \frac{1}{Q^2}\left[\frac{s^i}{i!} - \mathcal{P}_i(Q, s)\right],$$

and inversely,[a]

$$\mathcal{P}_i(Q, s) = \left[\frac{s^i}{i!} - Q^2\mathcal{P}_{i+2}(Q, s)\right].$$

Integration and differentiation have the following properties:

$$\frac{d\mathcal{P}_i(Q, s)}{ds} = \mathcal{P}_{i-1}(Q, s),$$

$$\int_0^s x^j \mathcal{P}_i(Q, x)dx = j!\sum_{k=0}^{j} \frac{(-1)^k}{(j-k)!} s^{j-k}\mathcal{P}_{i+k+1}(Q, s)$$

and in particular

$$\int_0^s \mathcal{P}_i(Q, x)dx = \mathcal{P}_{i+1}(Q, s).$$

The "multiply" property (for any integer m) is

$$\mathcal{P}_i(Q, ms) = m^i \mathcal{P}_i(mQ, s).$$

Thus, a very useful "doubling" rule is:

$$\mathcal{P}_i(Q, 2s) = 2^i \mathcal{P}_i(2Q, s).$$

There are the following "product" rules (they can be proved with the help of usual mathematical induction method):

[a] These expressions are very useful for saving computer time, because they allow us to calculate all $\mathcal{P}_i$-functions if series $\mathcal{P}_i$, with highest odd and even numbers are known.

$$\mathcal{P}_{2i}(Q_1,s)\cdot\mathcal{P}_{2j}(Q_2,s) = \frac{(Q_1+Q_2)^{2i+2j}}{2Q_1^{2i}Q_2^{2j}}\mathcal{P}_{2i+2j}(Q_1+Q_2,s)+ \\ + \frac{(Q_1-Q_2)^{2i+2j}}{2Q_1^{2i}Q_2^{2j}}\mathcal{P}_{2i+2j}(Q_1-Q_2,s)- \\ -\sum_{k=0}^{i-1}\frac{s^{2k}}{(2k)!}\left(\frac{Q_2}{Q_1}\right)^{2i-2k}\mathcal{P}_{2i+2j-2k}(Q_2,s)- \\ -\sum_{k=0}^{j-1}\frac{s^{2k}}{(2k)!}\left(\frac{Q_1}{Q_2}\right)^{2j-2k}\mathcal{P}_{2i+2j-2k}(Q_1,s);$$

$$\mathcal{P}_{2i+1}(Q_1,s)\cdot\mathcal{P}_{2j}(Q_2,s) = \frac{(Q_1+Q_2)^{2i+2j+1}}{2Q_1^{2i+1}Q_2^{2j}}\mathcal{P}_{2i+2j+1}(Q_1+Q_2,s)+ \\ + \frac{(Q_1-Q_2)^{2i+2j+1}}{2Q_1^{2i+1}Q_2^{2j}}\mathcal{P}_{2i+2j+1}(Q_1-Q_2,s)- \\ -\sum_{k=0}^{i-1}\frac{s^{2k+1}}{(2k+1)!}\left(\frac{Q_2}{Q_1}\right)^{2i-2k}\mathcal{P}_{2i+2j-2k}(Q_2,s)- \\ -\sum_{k=0}^{j-1}\frac{s^{2k}}{(2k)!}\left(\frac{Q_1}{Q_2}\right)^{2j-2k}\mathcal{P}_{2i+2j+1-2k}(Q_1,s);$$

$$\mathcal{P}_{2i+1}(Q_1,s)\cdot\mathcal{P}_{2j+1}(Q_2,s) = \frac{(Q_1+Q_2)^{2i+2j+2}}{2Q_1^{2i+1}Q_2^{2j+1}}\mathcal{P}_{2i+2j+2}(Q_1+Q_2,s)- \\ - \frac{(Q_1-Q_2)^{2i+2j+2}}{2Q_1^{2i+1}Q_2^{2j+1}}\mathcal{P}_{2i+2j+2}(Q_1-Q_2,s)- \\ -\sum_{k=0}^{i-1}\frac{s^{2k+1}}{(2k+1)!}\left(\frac{Q_2}{Q_1}\right)^{2i-2k}\mathcal{P}_{2i+2j+1-2k}(Q_2,s)- \\ -\sum_{k=0}^{j-1}\frac{s^{2k+1}}{(2k+1)!}\left(\frac{Q_1}{Q_2}\right)^{2j-2k}\mathcal{P}_{2i+2j+1-2k}(Q_1,s).$$

These "product" rules are very useful and were effectively used in the computer code HAMIL.RED for Lie operators calculations.

3 $\mathcal{D}$-FUNCTIONS

Let us introduce the functions $\mathcal{D}_i(Q_1, Q_2, s)$ as "double" series

$$\mathcal{D}_i(Q_1, Q_2, s) = s^i \sum_{j=0}^{\infty} \frac{1}{(2j+i)!} \sum_{k=0}^{j} (-Q_1^2 s^2)^{j-k} (-Q_2^2 s^2)^k.$$

The relations between $\mathcal{D}$-functions and usual trigonometrical functions are determined by the following expressions:

$$\mathcal{D}_0(Q_1, Q_2, s) = \frac{Q_1^2 \cos Q_1 s - Q_2^2 \cos Q_2 s}{Q_1^2 - Q_2^2},$$

$$\mathcal{D}_1(Q_1, Q_2, s) = \frac{Q_1 \sin Q_1 s - Q_2 \sin Q_2 s}{Q_1^2 - Q_2^2},$$

$$\mathcal{D}_2(Q_1, Q_2, s) = \frac{-\cos Q_1 s + \cos Q_2 s}{Q_1^2 - Q_2^2},$$

$$\mathcal{D}_3(Q_1, Q_2, s) = \frac{-\frac{\sin Q_1 s}{Q_1} + \frac{\sin Q_2 s}{Q_2}}{Q_1^2 - Q_2^2}$$

and etc. The constructions in the right parts of these expressions appear as a rule during the determination of Lie operators for magnets with skew quadrupole components. The usage of $\mathcal{D}$-functions allow us to simplify the computer analytical calculations and final formulae, and to eliminate the small denominators $Q_1^2 - Q_2^2$.

These functions have the following properties:

$$\mathcal{D}_i(0, 0, s) = \frac{s^i}{i!},$$

$$\mathcal{D}_i(Q_1, Q_2, 0) = \begin{cases} 0 & \text{if } i \neq 0; \\ 1 & \text{if } i = 0, \end{cases}$$

$$\mathcal{D}_i(Q_1, Q_2, s) = \mathcal{D}_i(Q_2, Q_1, s);$$

$$\mathcal{D}_i(Q, 0, s) = \mathcal{P}_i(Q, s).$$

The following recurrent expressions are valid:

$$\mathcal{D}_{i+2}(Q_1, Q_2, s) = \frac{\mathcal{P}_i(Q_2, s) - \mathcal{D}_i(Q_1, Q_2, s)}{Q_1^2} = \frac{\mathcal{P}_i(Q_1, s) - \mathcal{D}_i(Q_1, Q_2, s)}{Q_2^2}$$

and inversely,[b]

$$\mathcal{D}_i(Q_1, Q_2, s) = \mathcal{P}_i(Q_2, s) - Q_1^2 \mathcal{D}_{i+2}(Q_1, Q_2, s) =$$
$$= \mathcal{P}_i(Q_1, s) - Q_2^2 \mathcal{D}_{i+2}(Q_1, Q_2, s).$$

Integration and differentiation have the following properties:

$$\frac{d\mathcal{D}_i(Q_1, Q_2, s)}{ds} = \mathcal{D}_{i-1}(Q_1, Q_2, s),$$

$$\int_0^s x^j \mathcal{D}_i(Q_1, Q_2, x)dx = j! \sum_{k=0}^{j} \frac{(-1)^k}{(j-k)!} s^{j-k} \mathcal{D}_{i+k+1}(Q_1, Q_2, s)$$

and, in particular

$$\int_0^s \mathcal{D}_i(Q_1, Q_2, x)dx = \mathcal{D}_{i+1}(Q_1, Q_2, s).$$

The following expressions contain $\mathcal{P}$-functions only:

$$\mathcal{D}_i(Q_1, Q_2, s) = \frac{Q_1^2 \mathcal{P}_i(Q_1, s) - Q_2^2 \mathcal{P}_i(Q_2, s)}{Q_1^2 - Q_2^2},$$

$$\mathcal{D}_{i+2}(Q_1, Q_2, s) = -\frac{\mathcal{P}_i(Q_1, s) - \mathcal{P}_i(Q_2, s)}{Q_1^2 - Q_2^2}$$

and, in particular

$$\mathcal{D}_i(Q, Q, s) = \frac{1}{2}\left[s\mathcal{P}_{i-1}(Q, s) + (2-i)\mathcal{P}_i(Q, s)\right] \text{ for } i \geq 1,$$

$$\mathcal{D}_0(Q, Q, s) = \mathcal{P}_0(Q, s) - \frac{1}{2} Q^2 s \mathcal{P}_1(Q, s).$$

The following useful relations were used also into the REDUCE code:

---

[b] These expressions are very useful for computer time saving, because they allow to calculate all $\mathcal{D}_i$-functions if series $\mathcal{D}_i$ with the highest odd and even indices are known. Naturally, the $\mathcal{P}$-functions must be calculated as well.

$$\mathcal{D}_0(Q_1, Q_2, s) = \mathcal{P}_0\left(\frac{Q_1+Q_2}{2}, s\right)\mathcal{P}_0\left(\frac{Q_1-Q_2}{2}, s\right) - $$

$$- \frac{Q_1^2+Q_2^2}{4}\mathcal{P}_1\left(\frac{Q_1+Q_2}{2}, s\right)\mathcal{P}_1\left(\frac{Q_1-Q_2}{2}, s\right),$$

$$\mathcal{D}_1(Q_1, Q_2, s) = \frac{1}{2}\left[\mathcal{P}_0\left(\frac{Q_1+Q_2}{2}, s\right)\mathcal{P}_1\left(\frac{Q_1-Q_2}{2}, s\right) + \right.$$

$$\left. + \mathcal{P}_1\left(\frac{Q_1+Q_2}{2}, s\right)\mathcal{P}_0\left(\frac{Q_1-Q_2}{2}, s\right)\right],$$

$$\mathcal{D}_2(Q_1, Q_2, s) = \frac{1}{2}\mathcal{P}_1\left(\frac{Q_1+Q_2}{2}, s\right)\mathcal{P}_1\left(\frac{Q_1-Q_2}{2}, s\right),$$

$$\mathcal{D}_1(Q_1+Q_2, Q_1-Q_2, s) = \frac{1}{2}\left[\mathcal{P}_0(Q_1, s)\mathcal{P}_1(Q_2, s) + \mathcal{P}_0(Q_2, s)\mathcal{P}_1(Q_1, s)\right],$$

$$\mathcal{D}_2(Q_1+Q_2, Q_1-Q_2, s) = \frac{1}{2}\mathcal{P}_1(Q_1, s)\mathcal{P}_1(Q_2, s).$$

4 REDUCE CODE FOR OPERATOR DETERMINATION

Computer code HAMIL.RED was created for the calculation of analytical expressions of the orbital and spin Lie operators. We restrict calculations to the sextupole order only for orbital and spin motions, but the code for calculations of next order Lie operators without serious problems can be modified.

The expansion of the vector potential in power series in coordinates and expressions of orbital linear transformation matrices was used as input data for this code. The scenario of the code HAMIL.RED is as follows. Firstly, the code reads expressions of the vector potential and calculates terms of magnetic field and Hamiltonian, separated by the order of the variables in six-dimensional phase space. The following code reads orbital matrices and calculates spin linear matrices. Coefficients of orbital and spin Lie operators are calculated at the next stage. Finally the code checks the expressions obtained.

The expansion of the vector potential $\vec{A}$ was written in the natural frame.[6] The terms of the 3-rd power of the orbital vector $\vec{Z} = (x, p_x, z, p_z, \sigma, p_\sigma)$ components were used in the expressions for the components of $\vec{A}$. Therefore, the sextupole terms will be taken into account for the Hamiltonian, including all edge-effects (the corresponding derivatives with respect to longitudinal coordinates are preserved).

Only one limitation was used: the orbit was assumed to be without torsion (the orbit is piecewise planar!).

The following notations are used for the dimensionless magnetic field $\vec{B} \equiv e\vec{B}/E_0$ (E_0 is the fixed particle energy) on the reference orbit ($x = z = 0$):

$K = B_z$ – the curvature in x-direction,
$g = \frac{\partial B_z}{\partial x}$ – the magnetic field gradient,
$q = \frac{1}{2}\left(\frac{\partial B_x}{\partial x} - \frac{\partial B_z}{\partial z}\right)$ – the skew-gradient,
$m_x = \partial^2 B_z/\partial x^2$ – the sextupole moment of the magnetic field,
$m_z = \partial^2 B_z/\partial x \partial z$ – the skew-sextupole moment.
Primes are used for the definition of the s-derivatives.

These are the following expressions for the components of the vector potential $\vec{A}(h = 1 + Kx)$:

$$
\begin{aligned}
A_x = & -\frac{1}{2}B_s z - \frac{1}{2}B_x' xz - \frac{1}{4}B_z' z^2 - \frac{1}{4}(g' - KB_z')xz^2 - \\
& -\frac{1}{4}\left(q' - \frac{1}{2}B_s''\right)x^2 z + \frac{1}{12}\left(q' + \frac{1}{2}B_s''\right)z^3, \\
A_z = & \frac{1}{2}B_s x + \frac{1}{2}B_z' xz + \frac{1}{4}B_x' x^2 + \frac{1}{4}(g' - KB_z')x^2 z - \\
& -\frac{1}{4}\left(q' + \frac{1}{2}B_s''\right)xz^2 + \frac{1}{12}\left(q' - \frac{1}{2}B_s''\right)x^3, \\
h \cdot A_s = & -B_z x + B_x z - \frac{1}{2}(g + KB_z)x^2 + \frac{1}{2}gz^2 + qxz - \\
& -\frac{1}{6}(m_x + 2Kg)x^3 + \frac{1}{6}m_z z^3 - \frac{1}{2}\left(m_z - Kq + \frac{1}{2}B_x''\right)x^2 z + \\
& +\frac{1}{2}\left(m_x + Kg + \frac{1}{2}B_z''\right)xz^2.
\end{aligned}
$$

These equations allow to find the components of the magnetic field and the total Hamiltonian:

$$
\mathcal{H} = c\sqrt{\left(\vec{P} - \frac{e}{c}\vec{A}\right)^2 + m^2c^2} + \vec{\Omega}\vec{n}
$$

in the form of series over Z_i. The following abbreviations have been used: e, m and $\vec{n}$ are the charge of the particle, its rest mass and spin vector respectively, c is velocity of light, $\vec{P}$ is canonical momentum and $\vec{\Omega}$ is a spin precession frequency.[7]

Let us write the results for the total Hamiltonian as a sum of the corresponding polynomials $\mathcal{H}_i$ and $\vec{\Omega} = \vec{\omega}^{(0)} + \vec{\omega}^{(1)} + \vec{\omega}^{(2)}$:

$$
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2,
$$

where[c]

$$\mathcal{H}_0 = \frac{1}{2}\left(p_x^2 + p_z^2 + B_s\left(p_x z - x p_z\right) + \frac{1}{4}B_s^2\left(x^2+z^2\right) - 2Kxp_\sigma + \left(K^2+g\right)x^2 - \right.$$

$$\left. - g z^2\right) - qxz + \vec{\omega}^{(0)}\vec{n}$$

$$\equiv h_{ij}^{(0)} Z_i Z_j + \omega_\alpha^{(0)} n_\alpha,$$

$$\mathcal{H}_1 = \frac{1}{6}\left(2Kg + m_x\right)x^3 + \frac{1}{2}\left(m_z - Kq + \frac{1}{2}B_s''\right)x^2 z - \frac{1}{8}B_s^2\left(x^2+z^2\right)p_\sigma +$$

$$+ \frac{1}{2}Kxp_x^2 - \frac{1}{2}\left(m_x + Kg + \frac{1}{2}B_z''\right)xz^2 - \frac{1}{2}B_z' xzp_z + \frac{1}{2}Kxp_z^2 + \frac{1}{2}B_s x p_x p_\sigma -$$

$$- \frac{1}{2}\left(p_x^2 + p_z^2\right)p_\sigma + \frac{1}{4}B_z' p_x z^2 - \frac{1}{2}B_s p_x z p_\sigma - \frac{1}{6}m_z z^3 + \vec{\omega}^{(1)}\vec{n}$$

$$\equiv h_{ijk}^{(1)} Z_i Z_j Z_k + \omega_{\alpha i}^{(1)} n_\alpha Z_i,$$

$$\mathcal{H}_2 = \vec{\omega}^{(2)}\vec{n}$$

$$\equiv \omega_{\alpha ij}^{(2)} n_\alpha Z_i Z_j$$

and ($a = 1.159\ldots \cdot 10^{-3}$ is the dimensionless anomalous magnetic momentum of the electron)

$$\vec{\omega}^{(0)} = -B_z\left(a\gamma_0 + \frac{a\gamma_0}{2} + \frac{1}{2\gamma_0^2}\right)\vec{e}_z - B_s\left(1 + a + \frac{1}{2\gamma_0^2}\right)\vec{e}_\tau,$$

$$\vec{\omega}^{(1)} = \left\{\left(\frac{1}{2}B_s' - q\right)(1+a\gamma_0)x + B_s a(1-\gamma_0)p_x + \left[\frac{1}{2}B_s^2 a(\gamma_0 - 1) - \right.\right.$$

$$\left.\left. - g(1+a\gamma_0)\right]z\right\}\vec{e}_x +$$

$$+ \left\{-\left[\frac{1}{2}B_s^2 a(1-\gamma_0) + (KB_z + g)(1+a\gamma_0)\right]x + \right.$$

$$\left. + \left(\frac{1}{2}B_s' + q\right)(1+a\gamma_0)z + B_s a(\gamma_0 - 1)p_z + B_z p_\sigma\right\}\vec{e}_z +$$

$$+ \left\{-B_z'(1+a)z + B_z a(\gamma_0 - 1)p_z + B_s(1+a)p_\sigma\right\}\vec{e}_\tau,$$

[c] All Latin indices $i, j, \ldots$ are equal to $1, 2, \ldots, 6$ and correspond to components of the orbital vector $\vec{Z}$; all Greek indices $\alpha, \beta, \ldots$ correspond to x, z, τ and the standard rule is used for the summation over the mute indices.

$$\vec{\omega}^{(2)} = \left\{\frac{1}{2}(m_z - Kq)(1+a\gamma_0)x^2 - (m_x + Kg)(1+a\gamma_0)xz - \left(\frac{1}{2}B_s' - q\right)xp_\sigma + \right.$$

$$\left. + B_z' a\gamma_0 p_x z + B_z a\gamma_0 p_x p_z - \frac{1}{2}m_z(1+a\gamma_0)zp_\sigma\right\}\vec{e}_x +$$

$$+ \left\{-\frac{1}{2}m_x(1+a\gamma_0)x^2 + (Kq - m_z)(1+a\gamma_0)xz + (KB_z + g)xp_\sigma - \right.$$

$$- \frac{1}{2}B_z(1+a\gamma_0)p_x^2 + \frac{1}{2}(Kg + m_x + B_z'')(1+a\gamma_0)z^2 + B_z' a\gamma_0 z p_z -$$

$$\left. - \left(\frac{1}{2}B_s' + q\right)zp_\sigma + \frac{1}{2}B_z(a\gamma_0 - 1)p_z^2 - B_z p_\sigma^2\right\}\vec{e}_z +$$

$$+ \left\{-\frac{1}{2}\left[\frac{1}{4}B_s^3(2a\gamma_0 + 1) + \left(q' - \frac{1}{2}B_s''\right)\right]x^2 + \left(q - \frac{1}{2}B_s'\right)a\gamma_0 x p_x - \right.$$

$$- g'xz + \left[ga\gamma_0 + \frac{1}{2}B_s^2(2a\gamma_0 + 1)\right]xp_z - \frac{1}{2}B_s(2a\gamma_0 + 1)p_x^2 -$$

$$- \left[\frac{1}{2}B_s^2(2a\gamma_0 + 1) - ga\gamma_0\right]p_x z - \frac{1}{2}\left[\frac{1}{4}B_s^3(2a\gamma + 1) - \right.$$

$$\left. - \left(q' + \frac{1}{2}B_s''\right)\right]z^2 - \left(q + \frac{1}{2}B_s'\right)a\gamma_0 z p_z - \frac{1}{2}B_s(2a\gamma_0 + 1)p_z^2 +$$

$$\left. + B_z' z p_\sigma - B_s p_\sigma^2\right\}\vec{e}_\tau.$$

The next HAMIL.RED stage is the calculation of the Lie operators. As it is known, the operators of the linear transformations are simply the matrices $\mathcal{A}$ for orbital and $\mathcal{S}$ for spin motion. For each type of collider elements the first of them is included into the code "by hand". The matrices $\mathcal{S}$ are calculated within the code according to the formula[2] ($\omega_0 = |\vec{\omega}^{(0)}|$):

$$\mathcal{S}_{ij}(\theta) = \delta_{ij} + \mathcal{P}_1(\omega_0, \theta)e_{ijk}\omega_k^{(0)} + \mathcal{P}_2(\omega_0, \theta)\left[\omega_0^2\delta_{ij} - \omega_i^{(0)}\omega_j^{(0)}\right].$$

After that the code calculates all coefficients $\mathcal{F}_{ijk}$, $\mathcal{W}_{\alpha i}^{(1)}$ and $\mathcal{W}_{\alpha ij}^{(2)}$ for orbital and spin Lie operators for all element types:[4]

$$\mathcal{F}_{ijk}(\theta) = \int_0^\theta d\theta' h^{(1)}_{lmn} \mathcal{A}_{li}(\theta')\mathcal{A}_{mj}(\theta')\mathcal{A}_{nk}(\theta'),$$

$$\mathcal{W}^{(1)}_{\alpha i}(\theta) = \int_0^\theta d\theta' \mathcal{S}^{-1}_{\alpha\beta}(\theta')\omega^{(1)}_{\beta j}\mathcal{A}_{ji}(\theta'),$$

$$\begin{aligned}\mathcal{W}^{(2)}_{\alpha ij}(\theta) = \int_0^\theta d\theta' \Big(& \mathcal{S}^{-1}_{\alpha\beta}(\theta')\omega^{(2)}_{\beta kl}\mathcal{A}_{ki}(\theta')\mathcal{A}_{lj}(\theta') + \\ & + \frac{1}{2} e_{\alpha\beta\gamma}\mathcal{W}^{(1)}_{\beta i}(\theta')\mathcal{S}^{-1}_{\gamma\lambda}(\theta')\omega^{(1)}_{\lambda k}\mathcal{A}_{kj}(\theta') + \\ & + \mathcal{S}^{-1}_{\alpha\beta}(\theta')\omega^{(1)}_{\beta k}\mathcal{A}_{kl}(\theta') J_{lm}\mathcal{F}_{mij}(\theta')\Big)\end{aligned}$$

and, as is known,

$$J = \begin{pmatrix} \mathcal{J} & 0 & 0 \\ 0 & \mathcal{J} & 0 \\ 0 & 0 & \mathcal{J} \end{pmatrix} \quad \text{and} \quad \mathcal{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

The last steps of the HAMIL.RED are tests of the results for Lie operators. The "doubling" rule is used for these calculations. The rule is based on the comparison of two different methods for the operator calculations of the element with double length: a) the substitution of value $2L$ into the results instead of value L and b) "unification" of two elements with length L for each of them (indices (u) and (v)) corresponding to one element (index (w)). The Lie operator transformation formulae are used for this "unification":[4]

$$\begin{aligned}
\mathcal{A}^{(w)}_{ij} &= \mathcal{A}^{(v)}_{ik}\mathcal{A}^{(u)}_{kj}, \\
\mathcal{F}^{(w)}_{ijk} &= \mathcal{F}^{(u)}_{ijk} + \mathcal{F}^{(v)}_{lmn}\mathcal{A}^{(u)}_{li}\mathcal{A}^{(u)}_{mj}\mathcal{A}^{(u)}_{nk}, \\
\mathcal{S}^{(w)}_{\alpha\beta} &= \mathcal{S}^{(v)}_{\alpha\gamma}\mathcal{S}^{(u)}_{\gamma\beta}, \\
\mathcal{W}^{(1)}_{\alpha i} &= \mathcal{U}^{(1)}_{\alpha i} + \mathcal{S}^{(u)^{-1}}_{\alpha\beta}\mathcal{V}^{(2)}_{\beta j}\mathcal{A}^{(u)}_{ji}, \\
\mathcal{W}^{(2)}_{\alpha ij} &= \mathcal{U}^{(2)}_{\alpha ij} + \mathcal{S}^{(u)^{-1}}_{\alpha\beta}\mathcal{V}^{(2)}_{\beta kl}\mathcal{A}^{(u)}_{ki}\mathcal{A}^{(u)}_{lj} + \\
&\quad + \frac{1}{2} e_{\alpha\beta\gamma}\mathcal{U}^{(1)}_{\beta i}\mathcal{S}^{(u)^{-1}}_{\gamma\lambda}\mathcal{V}^{(1)}_{\lambda k}\mathcal{A}^{(u)}_{kj} + \\
&\quad + \mathcal{S}^{(u)^{-1}}_{\alpha\beta}\mathcal{V}^{(1)}_{\beta k}\mathcal{A}^{(u)}_{kl} J_{lm}\mathcal{F}^{(u)}_{mij}.
\end{aligned}$$

All s-derivatives of the magnetic field or its gradient are considered in the case of EDGE element only. They are treated as delta-functions of s ($B' \equiv B\delta(s - s_{\rm in})$ for entrance or $B' \equiv -B\delta(s - s_{\rm out})$ for exit). For this reason the integrals from the first s-derivatives are taken as equal to the field steps (ΔB_x, ΔB_z and etc.) or its gradient steps (Δg, Δq and etc.). The second s-derivatives are replaced by the first, using integration by parts:

$$\int_{s-\epsilon}^{s+\epsilon} B'' Z_i Z_j ds' = B' Z_i Z_j \Big|_{s-\epsilon}^{s+\epsilon} - \int_{s-\epsilon}^{s+\epsilon} B'(Z_i Z_j)' ds'.$$

5 MATRICES, LIE OPERATORS

The orbital and spin Lie operators for two types of collider elements — magnets with homogeneous vertical field and magnets with quadrupole and skew quadrupole components are presented in this part. We have chosen these types as examples, but all types which are used in modern colliders were calculated. The first one allows us to compare results for orbital Lie operators (using $\mathcal{P}$- and $\mathcal{D}$-functions) and results of previous authors ([3] for example). The second example demonstrates complicated final expressions which must be programmed for real numerical calculations, and shows the advantages of using $\mathcal{P}$- and $\mathcal{D}$-functions.

All orbital and spin Lie operators which are not included in this list equal zero. For all $\mathcal{P}(Q, s)$- and $\mathcal{D}(Q_1, Q_2, s)$-functions the second argument equals L and is omitted for simplicity.

Let us ascribe different indices to the spin second order Lie operators in the following cases:

- a – the sextupole order term $\vec{\omega}^{(2)}$ taken into account in the expansion of the spin precession frequency $\vec{\Omega}$;
- b – the term taken into account caused by the orbital motion nonlinearity (the "product" $\vec{\omega}^{(1)} \cdot \mathcal{F}_{ijk}$);
- c – the product $[\vec{\omega}^{(1)}, \vec{\omega}^{(1)}]$ taken into account.

In practice the sum of all these terms is calculated. Sometimes, the separation is useful for investigations of different terms influence on nonlinear spin dynamics.

5.1 *Bending magnet with homogeneous field*

(A) Parameters length L, magnetic field $K = \frac{e}{E_0} B_z$.

(B) The orbital matrix:

$$
\mathcal{A} = \begin{pmatrix}
\mathcal{P}_0(K) & \mathcal{P}_1(K) & 0 & 0 & 0 & K\mathcal{P}_2(K) \\
-K^2\mathcal{P}_1(K) & \mathcal{P}_0(K) & 0 & 0 & 0 & K\mathcal{P}_1(K) \\
0 & 0 & 1 & L & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
-K\mathcal{P}_1(K) & -K\mathcal{P}_2(K) & 0 & 0 & 0 & -K^2\mathcal{P}_3(K) \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}.
$$

(C) The vector of the distorted orbit, which is connected with synchrotron radiation losses ($c_1 = \frac{2}{3} r_0 \gamma^3$, where r_0 is the classical electron radius. Since $c_1 = 0.14077848 \cdot 10^{-11} \cdot E^3_{[\mathrm{MeV}]}$):

$$
(-c_1 K^3 \mathcal{P}_3(K),\ -c_1 K^3 \mathcal{P}_2(K),\ 0,\ 0,\ c_1 K^4 \mathcal{P}_4(K),\ -c_1 K^2 L).
$$

(D) The spin matrix

$$
\mathcal{S} = \begin{pmatrix}
\mathcal{P}_0(a\gamma K) & 0 & -a\gamma K \mathcal{P}_1(a\gamma K) \\
0 & 1 & 0 \\
a\gamma K \mathcal{P}_1(a\gamma K) & 0 & \mathcal{P}_0(a\gamma K)
\end{pmatrix}.
$$

(E) The orbital Lie operators:

$$
\mathcal{F}_{111} = \frac{3}{4} K^3 \left[-\mathcal{P}_1(3K) + \mathcal{P}_1(K)\right],
$$

$$
\mathcal{F}_{112} = \frac{1}{4} K \left[\mathcal{P}_0(3K) - \mathcal{P}_0(K)\right],
$$

$$
\mathcal{F}_{116} = \frac{3}{4} K^2 \left[\mathcal{P}_1(3K) - \mathcal{P}_1(K)\right],
$$

$$
\mathcal{F}_{122} = \frac{1}{4} K \left[3\mathcal{P}_1(3K) + \mathcal{P}_1(K)\right],
$$

$$
\mathcal{F}_{126} = \frac{1}{4} \left[\mathcal{P}_0(K) - \mathcal{P}_0(3K)\right],
$$

$$
\mathcal{F}_{133} = K\mathcal{P}_1(K),
$$

$$\mathcal{F}_{166} = \frac{3}{4}K\left[\mathcal{P}_1(K) - \mathcal{P}_1(3K)\right],$$

$$\mathcal{F}_{222} = \frac{3}{4}K\left[3\mathcal{P}_2(3K) + \mathcal{P}_2(K)\right],$$

$$\mathcal{F}_{226} = -\frac{1}{4}\left[3\mathcal{P}_1(3K) + \mathcal{P}_1(K)\right],$$

$$\mathcal{F}_{244} = K\mathcal{P}_2(K),$$

$$\mathcal{F}_{266} = \frac{1}{4}K\left[\mathcal{P}_2(K) - 9\mathcal{P}_2(3K)\right],$$

$$\mathcal{F}_{446} = -\mathcal{P}_1(K),$$

$$\mathcal{F}_{666} = \frac{3}{4}\left[\mathcal{P}_1(3K) - \mathcal{P}_1(K)\right],$$

(F) The spin Lie operators:

$$\mathcal{W}^{(1)}_{x4} = a^2\gamma^2K^2\mathcal{P}_2(a\gamma K),$$

$$\mathcal{W}^{(1)}_{z1} = -(a\gamma+1)K^2\mathcal{P}_1(K),$$

$$\mathcal{W}^{(1)}_{z2} = -(a\gamma+1)K^2\mathcal{P}_2(K),$$

$$\mathcal{W}^{(1)}_{z6} = K\left[(a\gamma+1)\mathcal{P}_1(K) - a\gamma L\right],$$

$$\mathcal{W}^{(1)}_{\tau4} = a\gamma K\mathcal{P}_1(a\gamma K);$$

$$\mathcal{W}^{(2.a)}_{x14} = \frac{a\gamma}{2}K^3\left[(a\gamma-1)\mathcal{P}_2((a\gamma-1)K) - (a\gamma+1)\mathcal{P}_2((a\gamma+1)K)\right],$$

$$\mathcal{W}^{(2.a)}_{x24} = a\gamma K\left[\mathcal{P}_1((a\gamma-1)K) + \mathcal{P}_1((a\gamma+1)K)\right],$$

$$\mathcal{W}^{(2.a)}_{x46} = \frac{a\gamma}{2}K^2\left[(a\gamma+1)\mathcal{P}_2((a\gamma+1)K) - (a\gamma-1)\mathcal{P}_2((a\gamma-1)K)\right],$$

$$\mathcal{W}^{(2.a)}_{z11} = -(a\gamma+1)K^5\mathcal{P}_3(2K),$$

$$\mathcal{W}^{(2.a)}_{z12} = (a\gamma+1)K^3\mathcal{P}_2(2K),$$

$$\mathcal{W}_{z16}^{(2.a)} = K^2\left[2(a\gamma+1)K^2\mathcal{P}_3(2K)+\mathcal{P}_1(K)\right],$$

$$\mathcal{W}_{z22}^{(2.a)} = -(a\gamma+1)K^3\mathcal{P}_3(2K),$$

$$\mathcal{W}_{z26}^{(2.a)} = K^2\left[\mathcal{P}_2(K)-(a\gamma+1)\mathcal{P}_2(2K)\right],$$

$$\mathcal{W}_{z44}^{(2.a)} = \frac{a\gamma-1}{2}KL,$$

$$\mathcal{W}_{z66}^{(2.a)} = -K\left[(a\gamma+1)K^2\mathcal{P}_3(2K)+\mathcal{P}_1(K)\right],$$

$$\mathcal{W}_{\tau14}^{(2.a)} = \frac{a\gamma}{2}K^2\left[\mathcal{P}_1((a\gamma-1)K)-\mathcal{P}_1((a\gamma+1)K)\right],$$

$$\mathcal{W}_{\tau24}^{(2.a)} = \frac{a\gamma}{2}K^2\left[(a\gamma-1)\mathcal{P}_2((a\gamma-1)K)+(a\gamma+1)\mathcal{P}_2((a\gamma+1)K)\right],$$

$$\mathcal{W}_{\tau46}^{(2.a)} = \frac{a\gamma}{2}K\left[\mathcal{P}_1((a\gamma+1)K)-\mathcal{P}_1((a\gamma-1)K)\right],$$

$$\mathcal{W}_{z11}^{(2.b)} = 2(a\gamma+1)K^5\mathcal{P}_3(2K),$$

$$\mathcal{W}_{z12}^{(2.b)} = -2(a\gamma+1)K^3\mathcal{P}_2(2K),$$

$$\mathcal{W}_{z16}^{(2.b)} = -4(a\gamma+1)K^4\mathcal{P}_3(2K),$$

$$\mathcal{W}_{z22}^{(2.b)} = \frac{a\gamma+1}{2}\left[\mathcal{P}_1(2K)-2\mathcal{P}_1(K)+L\right],$$

$$\mathcal{W}_{z26}^{(2.b)} = 2(a\gamma+1)K^2\mathcal{P}_2(2K),$$

$$\mathcal{W}_{z44}^{(2.b)} = (a\gamma+1)K^3\mathcal{P}_3(K),$$

$$\mathcal{W}_{z66}^{(2.b)} = 2a^2(a\gamma+1)K^3\mathcal{P}_3(2K),$$

$$\mathcal{W}_{x14}^{(2.c)} = \frac{(a\gamma-1)(a\gamma+1)^2}{4}K^3\left[\mathcal{P}_2((a\gamma-1)K)-\mathcal{P}_2((a\gamma+1)K)\right],$$

$$\mathcal{W}_{x24}^{(2.c)} = \frac{a\gamma+1}{4}K\left[(a\gamma+1)\mathcal{P}_1((a\gamma-1)K)+(a\gamma-1)\mathcal{P}_1((a\gamma+1)K)-\right.$$

$$\left.-2a\gamma\mathcal{P}_1(a\gamma K)\right],$$

$$\mathcal{W}_{x46}^{(2.c)} = \frac{1}{4}K^2 \Big\{(a\gamma - 1)(a\gamma + 1)^2 \left[\mathcal{P}_2((a\gamma + 1)K) - \mathcal{P}_2((a\gamma - 1)K)\right] +$$

$$+2a^2\gamma^2 \left[\mathcal{P}_2(a\gamma K) - L\mathcal{P}_1(a\gamma K)\right]\Big\},$$

$$\mathcal{W}_{z44}^{(2.c)} = \frac{1}{2}a^3\gamma^3 K^3 \mathcal{P}_3(a\gamma K),$$

$$\mathcal{W}_{\tau 14}^{(2.c)} = \frac{a\gamma + 1}{4}K^2 \left[(a\gamma + 1)\mathcal{P}_1((a\gamma - 1)K) - (a\gamma - 1)\mathcal{P}_1((a\gamma + 1)K) -\right.$$

$$\left.-2\mathcal{P}_1(K)\right],$$

$$\mathcal{W}_{\tau 24}^{(2.c)} = \frac{a\gamma + 1}{4}K^2 \Big\{-(a^2\gamma^2 - 1)\left[\mathcal{P}_2((a\gamma - 1)K) + \mathcal{P}_2((a\gamma + 1)K)\right] +$$

$$+2a\left[a^2\gamma^2\mathcal{P}_2(a\gamma K) - \mathcal{P}_2(K)\right]\Big\},$$

$$\mathcal{W}_{\tau 46}^{(2.c)} = \frac{1}{4}K \Big\{(a\gamma + 1)\left[(a\gamma - 1)\mathcal{P}_1((a\gamma + 1)K) - (a\gamma + 1)\mathcal{P}_1((a\gamma - 1)K) +\right.$$

$$\left.+2\mathcal{P}_1(K)\right] - 2a\gamma\left[L\mathcal{P}_0(a\gamma K) - \mathcal{P}_1(a\gamma K)\right] - 2a^3\gamma^3\mathcal{P}_3(a\gamma K)\Big\}.$$

5.2 *Combined-functions magnet with skew-quadrupole*

(A) Parameters: length L and the standard values K, g and q. Then one can introduce:

$$Q_{1,2}^2 = \frac{K^2 \pm \sqrt{(K^2 + 2g)^2 + 4q^2}}{2}$$

(B) The orbital matrix $\mathcal{A}$ (the arguments of all $\mathcal{D}$-functions are Q_1, Q_2, L and for all $\mathcal{P}$-functions are Q_2, L):

$$\mathcal{A}_{11} = 1 - Q_1^2(Q_1^2 + g)\mathcal{D}_4 - (K^2 + g)\mathcal{P}_2,$$

$$\mathcal{A}_{12} = L - Q_1^2(Q_1^2 + g)\mathcal{D}_5 - (K^2 + g)\mathcal{P}_3,$$

$$\mathcal{A}_{13} = q(Q_1^2\mathcal{D}_4 + \mathcal{P}_2),$$

$$\mathcal{A}_{14} = q(Q_1^2\mathcal{D}_5 + \mathcal{P}_3),$$

$$\mathcal{A}_{16} = K\left[(Q_1^2 + g)\mathcal{D}_4 + \mathcal{P}_2\right],$$

$$\mathcal{A}_{21} = -(K^2 + g)L + Q_1^4(Q_1^2 + g)\mathcal{D}_5 + \left[q^2 + (K^2 + g)^2\right]\mathcal{P}_3,$$

$$\mathcal{A}_{22} = \mathcal{A}_{11},$$

$$\mathcal{A}_{23} = q(L - Q_1^4\mathcal{D}_5 - K^2\mathcal{P}_3),$$

$$\mathcal{A}_{24} = \mathcal{A}_{13},$$

$$\mathcal{A}_{26} = K\mathcal{A}_{12},$$

$$\mathcal{A}_{31} = \mathcal{A}_{13},$$

$$\mathcal{A}_{32} = \mathcal{A}_{14},$$

$$\mathcal{A}_{33} = 1 + Q_1^2(Q_2^2 + g)\mathcal{D}_4 + g\mathcal{P}_2,$$

$$\mathcal{A}_{34} = L + Q_1^2(Q_2^2 + g)\mathcal{D}_5 + g\mathcal{P}_3,$$

$$\mathcal{A}_{36} = -qK\mathcal{D}_4,$$

$$\mathcal{A}_{41} = \mathcal{A}_{23},$$

$$\mathcal{A}_{42} = \mathcal{A}_{13},$$

$$\mathcal{A}_{43} = gL - Q_1^4(Q_1^2 + g)\mathcal{D}_5 + (q^2 + g^2)\mathcal{P}_3,$$

$$\mathcal{A}_{44} = \mathcal{A}_{33},$$

$$\mathcal{A}_{46} = K\mathcal{A}_{14},$$

$$\mathcal{A}_{51} = -\mathcal{A}_{26},$$

$$\mathcal{A}_{52} = -\mathcal{A}_{16},$$

$$\mathcal{A}_{53} = -\mathcal{A}_{46},$$

$$\mathcal{A}_{54} = -\mathcal{A}_{36},$$

$$\mathcal{A}_{55} = 1,$$

$$\mathcal{A}_{56} = -K^2\left[(Q_1^2 + g)\mathcal{D}_5 + \mathcal{P}_3\right],$$

$$\mathcal{A}_{66} = 1,$$

$$\mathcal{A}_{ij} = 0 \text{ for other } i, j.$$

(C) The vector of the distorted orbit is simply the seventh column of the total 6⊗7 orbital matrix $\mathcal{A}$:

$$\mathcal{A}_{17} = -c_1 K^3 \left[(Q_1^2 + g)\mathcal{D}_5 + \mathcal{P}_3 \right],$$

$$\mathcal{A}_{27} = -c_1 K^2 \mathcal{A}_{16},$$

$$\mathcal{A}_{37} = c_1 q K^3 \mathcal{D}_5,$$

$$\mathcal{A}_{47} = -c_1 K^2 \mathcal{A}_{36},$$

$$\mathcal{A}_{57} = c_1 K^4 \left[(Q_1^2 + g)\mathcal{D}_6 + \mathcal{P}_4 \right],$$

$$\mathcal{A}_{67} = -c_1 K^2 L,$$

(D) The spin matrix is the same as for bending magnet.

(E,F) The expressions for orbital and spin Lie operators in this case are very complicated and not shown here.

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