Symmetry properties of a symplectic transport matrix and Twiss parameterization of a fully coupled motion

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Twiss parameterization proposed by Courant and Snyder is a keystone of accelerator physics. Several authors have extended it later to the case of the fully coupled betatron motion and synchrobetatron motion of a coasting beam. A few proposals have been made as well how to construct a parameterization which is fully symmetric with respect to all three spatial degrees of freedom. The key point for each of them is to find a similarity transformation which turns the transport matrix into a block-diagonal form with 2×2 cells. In the present work, this approach has been considered in detail. It is based on the idea initially proposed by Mais and Ripken for transport matrix eigenvalue calculation only. It shows how to introduce a symmetric Twiss-like parameterization and an emittance concept for an arbitrary symplectic 6×6 matrix. The resulting parameterization can be reduced to the well-known Lebedev-Bogacz parameterization in case of 4×4 matrix. Special attention has been paid to the intrinsic ambiguity existing in the Twiss parameterization of a coupled motion.

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I. INTRODUCTION

Coupling is an integral part of particle dynamics in accelerators. It has been studied by various authors; an abundance of efficient and commonly used tools has been developed to predict and control coupled motion. Existing theories usually treat longitudinal degree of freedom differently from the transversal ones which is reasonable from a physical point of view. However, mathematically speaking, it is possible to develop a theory treating all degrees of freedom in a similar way. This idea is not entirely new; however, this approach implies the presence of a significantly larger number of symmetry properties than have been studied before. Such an approach will be developed in the present paper, but first, a quick overview of the matrix optics basics and existing theories should be done.

Particle coordinates in circular accelerators are usually described as excursions from the corresponding coordinates of a *reference particle* which follows the *design orbit*. They can be chosen in such a way that the coordinates No. 1, 3, and 5 correspond to the spatial offsets in horizontal, vertical, and longitudinal direction, respectively; the coordinates No. 2, 4, and 6 are their canonical conjugates. In the present paper, coordinate vector will be denoted by $\bar{\Xi}$.

When linear approximation is used, the coordinate vectors $\bar{\Xi}_1$ at azimuth s_1 and $\bar{\Xi}_2$ at azimuth s_2, respectively, are related through the transport matrix $\mathbf{M}$ of the lattice region between s_1 and s_2:

$$\bar{\Xi}_2 = \mathbf{M}\bar{\Xi}_1. \tag{1}$$

Depending on the problem, either the full vector $\bar{\Xi}$, or four, or two of its components may be considered. According to the dimensionality of the transport matrices, three different cases will be distinguished in the present paper:

$$\begin{aligned} &6 \times 6 \text{ case: } \bar{\Xi} = (x,\ p_x,\ y,\ p_y,\ z,\ p_z)^T, \\ &4 \times 4 \text{ case: } \bar{\Xi} = (x,\ p_x,\ y,\ p_y)^T, \\ &2 \times 2 \text{ case: } \bar{\Xi} = (x,\ p_x)^T. \end{aligned}$$

Subsequent beamline elements with transport matrices $\mathbf{M}_1, \mathbf{M}_2, \cdots, \mathbf{M}_N$ can be described as a single element with the following transport matrix (see e.g., [1]):

$$\mathbf{M} = \mathbf{M}_N \cdots \mathbf{M}_2 \mathbf{M}_1.$$

Therefore, in a periodic lattice, it is possible to find a matrix of a single period. In what follows, $\mathbf{M}$ will be assumed to represent the transport matrix of a period in a periodic lattice, unless otherwise specified.

For the 2×2 case, the well-known Twiss parameterization proposed by Courant and Snyder in [2] exists. It works also for the 4×4 and 6×6 cases when the

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horizontal, vertical, and longitudinal dynamics are uncoupled. Moreover, it works also for a coasting beam in a lattice with horizontal-longitudinal and/or vertical-longitudinal coupling, where by introducing horizontal and/or vertical *dispersion*, one may reduce the 6×6 to the 4×4 case.

There are several different approaches in the 4×4 case with the fully coupled motion. The most well-known theories have been proposed by Lebedev and Bogacz [3], Edwards and Teng [4], Mais and Ripken [5], Sagan and Rubin [6], and Wolski [7]. Each of them can be reduced to the parameterization proposed by Courant and Snyder if two degrees of freedom are uncoupled. Therefore, the parameterization for the 6×6 case being developed in the present paper, to be useful, requires to be reduced to one of them when one degree of freedom is decoupled from other two. The Lebedev-Bogacz parameterization had been chosen for this purpose.

Among the proposals of a symmetric 6×6 parameterization, the works by Mais and Ripken [8], Wolski [9], and Parzen [10] should be noted. The former suggests an approach to the calculation of the eigenvalues and eigenvectors of a symplectic 6×6 matrix. The other two propose the parameterization itself, but they present only the main idea: 3 degrees of freedom can be decoupled by turning the transport matrix into a block-diagonal form using a similarity transformation. Many important features and symmetry properties have been studied in detail in the present paper to provide a deeper explanation of the parameterization and enhance its applicability across most cases. Preliminary results have been presented in [11]. Python scripts used to illustrate the main formulas given in the present paper have been published in [12].

Although no existing machines necessarily require such a symmetric approach, having such a tool at our disposal and knowing its properties could potentially offer a lot of new opportunities. Possible applications are discussed, e.g., in [9,13].

The papers [2–7,9,10] mentioned above have been cited in the recently published exhaustive overview by Vanwelde *et al.* [14] as well. This shows the continuing interest in this topic, despite the fact that the Twiss parameterization first found its application in accelerator physics more than 60 years ago.

II. SYMPLECTIC CONJUGATION

Symplecticity is a property of a transport matrix $\mathbf{M}$ of a lattice region where particle motion is governed by a time-independent Hamiltonian. Mathematically, it means the following:

$$\mathbf{M}^T\mathbf{S}_6\mathbf{M}=\mathbf{S}_6, \tag{2}$$

where $\mathbf{S}_n$ with even n is a block-diagonal $n\times n$ matrix consisting of *S blocks*:

$$\mathbf{S}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}.$$

For an arbitrary 2×2 matrix $\mathbf{A}$, a *symplectic conjugated* matrix $\hat{\mathbf{A}}$ can be defined in the following way[1]:

$$\hat{\mathbf{A}}=-\mathbf{S}\mathbf{A}^T\mathbf{S}. \tag{3}$$

Symplectic conjugation has the following properties which may be obtained by direct calculation:

$$\begin{aligned}
&1.\ |\mathbf{A}|=1\Rightarrow\hat{\mathbf{A}}=\mathbf{A}^{-1}\\
&2.\ \mathbf{A}+\hat{\mathbf{A}}=(\mathrm{Tr}\,\mathbf{A})\mathbf{I}=(\mathrm{Tr}\,\hat{\mathbf{A}})\mathbf{I}\\
&3.\ \mathbf{A}\hat{\mathbf{A}}=\hat{\mathbf{A}}\mathbf{A}=|\mathbf{A}|\mathbf{I}\\
&4.\ (\alpha\mathbf{A}+\beta\mathbf{B})\hat{}=\alpha\hat{\mathbf{A}}+\beta\hat{\mathbf{B}}\\
&5.\ \widehat{\mathbf{A}\mathbf{B}}=\hat{\mathbf{B}}\hat{\mathbf{A}}\\
&6.\ \hat{\hat{\mathbf{A}}}=\mathbf{A}
\end{aligned}, \tag{4}$$

where $\mathbf{A}$ and $\mathbf{B}$ are arbitrary 2×2 matrices, α and β are numbers, $\mathbf{I}$ is a 2×2 identity matrix. $n\times n$ identity matrices with $n\neq 2$ will be denoted as $\mathbf{I}_n$.

Symplectic conjugation can be defined for an $n\times n$ matrix $\mathbf{A}_n$ with an arbitrary even n as well:

$$\hat{\mathbf{A}}_n=-\mathbf{S}_n{\mathbf{A}_n}^T\mathbf{S}_n.$$

The *block form* of $\mathbf{A}_n$ is

$$\mathbf{A}_n=\begin{pmatrix}\mathbf{A}_{11} & \mathbf{A}_{12} & \cdots & \mathbf{A}_{1\frac{n}{2}}\\ \mathbf{A}_{21} & \mathbf{A}_{22} & \cdots & \mathbf{A}_{2\frac{n}{2}}\\ \vdots & \vdots & \ddots & \vdots\\ \mathbf{A}_{\frac{n}{2}1} & \mathbf{A}_{\frac{n}{2}2} & \cdots & \mathbf{A}_{\frac{n}{2}\frac{n}{2}}\end{pmatrix},$$

where corresponding elements of $\mathbf{A}_n$ are combined into 2×2 blocks $\mathbf{A}_{ij}$. Then

$$\hat{\mathbf{A}}_n=\begin{pmatrix}\hat{\mathbf{A}}_{11} & \hat{\mathbf{A}}_{21} & \cdots & \hat{\mathbf{A}}_{\frac{n}{2}1}\\ \hat{\mathbf{A}}_{12} & \hat{\mathbf{A}}_{22} & \cdots & \hat{\mathbf{A}}_{\frac{n}{2}2}\\ \vdots & \vdots & \ddots & \vdots\\ \hat{\mathbf{A}}_{1\frac{n}{2}} & \hat{\mathbf{A}}_{2\frac{n}{2}} & \cdots & \hat{\mathbf{A}}_{\frac{n}{2}\frac{n}{2}}\end{pmatrix},$$

[1]This operation had been introduced in [2] and denoted by $\bar{\mathbf{A}}$.

however, only properties No. 4, 5, and 6 in Eq. (4) are met in general for $n > 2$.

So, according to the definitions given above, one can rewrite the symplectic condition [Eq. (2)]:

$$\mathbf{M}^{-1} = \hat{\mathbf{M}} \tag{5}$$

and express $\mathbf{M}$ and its inverse in the block form:

$$\begin{aligned} \mathbf{M} &= \begin{pmatrix} \mathbf{M}_{11} & \mathbf{M}_{12} & \mathbf{M}_{13} \\ \mathbf{M}_{21} & \mathbf{M}_{22} & \mathbf{M}_{23} \\ \mathbf{M}_{31} & \mathbf{M}_{32} & \mathbf{M}_{33} \end{pmatrix}, \\ \mathbf{M}^{-1} &= \begin{pmatrix} \hat{\mathbf{M}}_{11} & \hat{\mathbf{M}}_{21} & \hat{\mathbf{M}}_{31} \\ \hat{\mathbf{M}}_{12} & \hat{\mathbf{M}}_{22} & \hat{\mathbf{M}}_{32} \\ \hat{\mathbf{M}}_{13} & \hat{\mathbf{M}}_{23} & \hat{\mathbf{M}}_{33} \end{pmatrix}. \end{aligned} \tag{6}$$

III. RECURRENT MATRIX

According to [8], a sum of the transport matrix $\mathbf{M}$ and its inverse turned out to be extremely useful for eigenanalysis. It will be denoted by $\overleftrightarrow{\mathbf{M}}$ and referred to as *recurrent matrix*[2]:

$$\overleftrightarrow{\mathbf{M}} = \mathbf{M} + \mathbf{M}^{-1}.$$

According to [2], all the eigenvalues of $\mathbf{M}$ can be divided into pairs where the product of the pair components is equal to 1. Let λ_1 and λ_2 form such a pair, $\bar{\mathbf{v}}_1$ and $\bar{\mathbf{v}}_2$ be their eigenvectors, i.e.,

$$\begin{aligned} &\mathbf{M}\bar{\mathbf{v}}_1 = \lambda_1\bar{\mathbf{v}}_1 \\ &\mathbf{M}\bar{\mathbf{v}}_2 = \lambda_2\bar{\mathbf{v}}_2 \\ &\lambda_1\lambda_2 = 1 \end{aligned} \Rightarrow \begin{aligned} &\mathbf{M}^{-1}\bar{\mathbf{v}}_1 = \tfrac{1}{\lambda_1}\bar{\mathbf{v}}_1 = \lambda_2\bar{\mathbf{v}}_1 \\ &\mathbf{M}^{-1}\bar{\mathbf{v}}_2 = \tfrac{1}{\lambda_2}\bar{\mathbf{v}}_2 = \lambda_1\bar{\mathbf{v}}_2 \end{aligned},$$

then

$$\begin{aligned} (\mathbf{M} + \mathbf{M}^{-1})\bar{\mathbf{v}}_1 &= (\lambda_1 + \lambda_2)\bar{\mathbf{v}}_1 \\ (\mathbf{M} + \mathbf{M}^{-1})\bar{\mathbf{v}}_2 &= (\lambda_1 + \lambda_2)\bar{\mathbf{v}}_2 \end{aligned}.$$

With the following notation

$$\hat{\lambda} = \lambda_1 + \lambda_2,$$

these equations can be transformed to their final form:

$$\begin{aligned} \overleftrightarrow{\mathbf{M}}\bar{\mathbf{v}}_1 &= \hat{\lambda}\bar{\mathbf{v}}_1 \\ \overleftrightarrow{\mathbf{M}}\bar{\mathbf{v}}_2 &= \hat{\lambda}\bar{\mathbf{v}}_2 \end{aligned}. \tag{7}$$

This means that $\overleftrightarrow{\mathbf{M}}$ has at most three different eigenvalues, each of them is degenerated at least twice, because linearly independent eigenvectors $\bar{\mathbf{v}}_1$ and $\bar{\mathbf{v}}_2$ correspond to the same eigenvalue $\hat{\lambda}$. Also, there is one-to-one correspondence between the spectra of $\overleftrightarrow{\mathbf{M}}$ and $\mathbf{M}$.

Matrix $\mathbf{M}$ describes stable motion if and only if all its eigenvalues are equal to 1 by absolute value [2], therefore,

$$\hat{\lambda} = 2\,\mathrm{Re}\,\lambda_{1,2}. \tag{8}$$

IV. RECURRENT MATRIX EIGENVALUES

The method used in this paper is proposed in Appendix II of [8]. However, it involves the notation, which we will need later, so its description is given here.[3]

In what follows, matrix $\mathbf{M}$ and other 6×6 matrices derived from it will often be used in the block form introduced in Eq. (6). This allows splitting matrix equations into systems of three equations on 2×2 matrix blocks where all indices range over the values $\{1, 2, 3\}$. An important symmetry property is that usually the equations within such a system can be obtained from each other using left or right cyclic shift of all or part of the indices. Introducing a special index formalism will allow us to use only one equation instead of three. Moreover, it will significantly shorten the code in any programming language needed to implement the technique.

Arrows $\overleftarrow{\ }$ and $\overrightarrow{\ }$ over indices will denote left and right cyclic shifts over the $\{1, 2, 3\}$ set, respectively. A comprehensive table of values for these operators is presented below:

$$\begin{aligned} &\overleftarrow{1} = 3, \quad \overleftarrow{2} = 1, \quad \overleftarrow{3} = 2, \\ &\overrightarrow{1} = 2, \quad \overrightarrow{2} = 3, \quad \overrightarrow{3} = 1. \end{aligned}$$

In what follows, we will assume that the indices i, j range over the values $\{1, 2, 3\}$, unless otherwise specified.

According to Eq. (6), recurrent matrix $\overleftrightarrow{\mathbf{M}}$ can be expressed as follows:

$$\overleftrightarrow{\mathbf{M}} = \mathbf{M} + \mathbf{M}^{-1} = \begin{pmatrix} b_1\mathbf{I} & \mathbf{R}_3 & \hat{\mathbf{R}}_2 \\ \hat{\mathbf{R}}_3 & b_2\mathbf{I} & \mathbf{R}_1 \\ \mathbf{R}_2 & \hat{\mathbf{R}}_1 & b_3\mathbf{I} \end{pmatrix}, \tag{9}$$

where

[2]The term refers to the fact that $\mathbf{M}$ and $\mathbf{M}^{-1}$ perform the opposite transformations of the coordinate vector [see Eq. (1)]. Moreover, according to Eq. (2), $|\mathbf{M}| \neq 0$, therefore, $\mathbf{M}^{-1}$ always exists.

[3]Since the description of the method is given only in the Appendix of [8] and no further derivation is based on it, it lacks details important for the present study; notation system also differs significantly. Moreover, neither of the two techniques for recurrent matrix eigenvector calculation proposed further in [8] is similar to the method described in the next section.

$$\mathbf{R}_i = \mathbf{M}_{\bar{i}\bar{i}} + \hat{\mathbf{M}}_{\bar{i}\bar{i}}, \tag{10}$$

$$b_i = \mathrm{Tr}\,\mathbf{M}_{ii}. \tag{11}$$

Matrices $\mathbf{R}_i$ will be referred to as *R matrices*, the following notation will be used for their determinants:

$$d_i = |\mathbf{R}_i|. \tag{12}$$

Let $\bar{\mathbf{v}}$ be an eigenvector of the $\overleftrightarrow{\mathbf{M}}$ matrix. It can be split into three two-component column vectors $\bar{\mathbf{X}}$, $\bar{\mathbf{Y}}$, and $\bar{\mathbf{Z}}$:

$$\bar{\mathbf{v}} = \begin{pmatrix} \bar{\mathbf{X}} \\ \bar{\mathbf{Y}} \\ \bar{\mathbf{Z}} \end{pmatrix}.$$

Using the notation

$$a_{ij} = b_i - \hat{\lambda}_j, \tag{13}$$

matrix equation $\overleftrightarrow{\mathbf{M}}\bar{\mathbf{v}} = \hat{\lambda}\bar{\mathbf{v}}$ on $\overleftrightarrow{\mathbf{M}}$ eigenvectors can be written as follows:

$$\begin{aligned} a_{1j}\bar{\mathbf{X}} + \mathbf{R}_3\bar{\mathbf{Y}} + \hat{\mathbf{R}}_2\bar{\mathbf{Z}} &= \bar{\mathbf{0}} \\ \hat{\mathbf{R}}_3\bar{\mathbf{X}} + a_{2j}\bar{\mathbf{Y}} + \mathbf{R}_1\bar{\mathbf{Z}} &= \bar{\mathbf{0}}, \\ \mathbf{R}_2\bar{\mathbf{X}} + \hat{\mathbf{R}}_1\bar{\mathbf{Y}} + a_{3j}\bar{\mathbf{Z}} &= \bar{\mathbf{0}} \end{aligned} \tag{14}$$

where $\bar{\mathbf{0}}$ is a two-component zero column vector. There is at least one nonzero vector among $\bar{\mathbf{X}}$, $\bar{\mathbf{Y}}$, and $\bar{\mathbf{Z}}$. Let it be $\bar{\mathbf{Z}}$, then excluding $\bar{\mathbf{X}}$ and $\bar{\mathbf{Y}}$ one obtains

$$\begin{aligned} &(\mathbf{R}_2\mathbf{R}_3\mathbf{R}_1 + \hat{\mathbf{R}}_1\hat{\mathbf{R}}_3\hat{\mathbf{R}}_2)\bar{\mathbf{Z}} \\ &= (a_{1j}d_1 + a_{2j}d_2 + a_{3j}d_3 - a_{1j}a_{2j}a_{3j})\bar{\mathbf{Z}} \end{aligned}$$

or

$$a_{1j}d_1 + a_{2j}d_2 + a_{3j}d_3 - a_{1j}a_{2j}a_{3j} = t, \tag{15}$$

where

$$t = \mathrm{Tr}\,(\mathbf{R}_1\mathbf{R}_2\mathbf{R}_3). \tag{16}$$

Using a_{ij} definition from Eq. (13), one obtains an equation on the $\hat{\lambda}_j$:

$$\begin{aligned} &\hat{\lambda}_j{}^3 - (b_1 + b_2 + b_3)\hat{\lambda}_j{}^2 \\ &+ (b_1b_2 + b_2b_3 + b_1b_3 - d_1 - d_2 - d_3)\hat{\lambda}_j \\ &+ (b_1d_1 + b_2d_2 + b_3d_3 - b_1b_2b_3 - t) = 0. \end{aligned} \tag{17}$$

As it was mentioned above, matrix $\overleftrightarrow{\mathbf{M}}$ has at most three different eigenvalues. Therefore, its characteristic polynomial is a full square of a third degree polynomial with real coefficients obtained in Eq. (17), which will be denoted by $\hat{P}(\hat{\lambda})$:

$$\hat{P}(\hat{\lambda}) = \sqrt{|\overleftrightarrow{\mathbf{M}} - \hat{\lambda}\mathbf{I}_6|} = \hat{\lambda}^3 + B\hat{\lambda}^2 + C\hat{\lambda} + D, \tag{18}$$

where

$$\begin{aligned} B &= -(b_1 + b_2 + b_3) \\ C &= b_2b_3 + b_3b_1 + b_1b_2 - d_1 - d_2 - d_3\,. \\ D &= b_1d_1 + b_2d_2 + b_3d_3 - b_1b_2b_3 - t \end{aligned} \tag{19}$$

We will solve the cubic equation [Eq. (17)] using the Cardano formulas [15]. First, we transform it to the canonical form $y^3 + py + q = 0$ using the substitution $\hat{\lambda} = y - B/3$, where

$$p = C - \frac{B^2}{3}, \qquad q = \frac{2B^3}{27} - \frac{BC}{3} + D. \tag{20}$$

The quantity

$$Q = \left(\frac{p}{3}\right)^3 + \left(\frac{q}{2}\right)^2 \tag{21}$$

determines the set of Eq. (17) roots: (i) $Q > 0$: one real root and two complex conjugated roots. Then two of the three $\mathbf{M}$ eigenvalue pairs have nonzero imaginary part and do not belong to the unit circle. Therefore, the matrix $\mathbf{M}$ describes unstable motion. (ii) $Q = 0$: one real root of the multiplicity 1 and two of the multiplicity 2, or (if $p = q = 0$) one real root of the multiplicity 3. Then the matrix $\mathbf{M}$ has coincident eigenvalues. (iii) $Q < 0$: three real roots. If at least one of them exceeds 2 by absolute value, then the matrix $\mathbf{M}$ has eigenvalues outside the unit circle, therefore, the matrix $\mathbf{M}$ describes unstable motion.

So, the motion is stable only if all three roots of Eq. (17) are real and do not exceed 2 by absolute value. In what follows, we will restrict ourselves to this case only.

If $p \neq 0$, then the roots can be expressed as follows:

$$\begin{aligned} \hat{\lambda}_a &= 2r\cos\varphi - \tfrac{B}{3} \\ \hat{\lambda}_{b,c} &= r(-\cos\varphi \pm \sqrt{3}\sin\varphi) - \tfrac{B}{3} \end{aligned}, \tag{22}$$

where

$$r = -\mathrm{sgn}\,q \cdot \sqrt{-\frac{p}{3}}, \quad \varphi = \frac{1}{3}\arccos\left(\frac{|q|}{2}\sqrt{-\frac{27}{p^3}}\right).$$

If $p = 0$, then $q = 0$ and $\hat{\lambda}_a = \hat{\lambda}_b = \hat{\lambda}_c = -B/3$.

The proposed algorithm is quite straightforward, but it does not take the correspondence between the eigenvalues and degrees of freedom into account. Therefore, eigenvalues $\hat{\lambda}_{a,b,c}$ should be sorted and renamed into $\hat{\lambda}_{1,2,3}$ so that

$\hat{\lambda}_{1,2,3}$ corresponds to the horizontal (x), vertical (y), and longitudinal (z) motion, respectively. This can be done only after eigenvector calculation, but for convenience from now on we will assume that the eigenvalues have been already sorted. Sorting algorithm is described in Appendix A, it utilizes the notation introduced in the next section.

V. RECURRENT MATRIX EIGENVECTORS

Equation system (14) can be transformed into the following form (it is split into three subsystems to simplify the subsequent derivations):

$$\begin{aligned} c_{1j}\bar{\mathbf{Y}} &= \hat{\mathbf{V}}_{3j}\bar{\mathbf{X}} \\ c_{1j}\bar{\mathbf{Z}} &= \mathbf{V}_{2j}\bar{\mathbf{X}} \\ c_{2j}\bar{\mathbf{Z}} &= \hat{\mathbf{V}}_{1j}\bar{\mathbf{Y}} \\ c_{2j}\bar{\mathbf{X}} &= \mathbf{V}_{3j}\bar{\mathbf{Y}} \\ c_{3j}\bar{\mathbf{X}} &= \hat{\mathbf{V}}_{2j}\bar{\mathbf{Z}} \\ c_{3j}\bar{\mathbf{Y}} &= \mathbf{V}_{1j}\bar{\mathbf{Z}} \end{aligned}, \tag{23}$$

where

$$\mathbf{V}_{ij} = \hat{\mathbf{R}}_{\bar{i}}\hat{\mathbf{R}}_{\bar{i}} - a_{ij}\mathbf{R}_i, \qquad c_{ij} = a_{\bar{i}j}a_{\bar{i}j} - d_i. \tag{24}$$

If there is at least one nonzero c_{ij} for a given j then Eq. (23) gives two linearly independent eigenvectors for the corresponding eigenvalue $\hat{\lambda}_j$. Anyway, one may create three matrices consisting of the $\overleftrightarrow{\mathbf{M}}$ eigenvector columns and/or zero vectors (that solve the eigenvector equation as well):

$$\mathbf{V}_j = \begin{pmatrix} c_{1j}\mathbf{I} & \mathbf{V}_{3\bar{j}} & \hat{\mathbf{V}}_{2\bar{j}} \\ \hat{\mathbf{V}}_{3j} & c_{2\bar{j}}\mathbf{I} & \mathbf{V}_{1\bar{j}} \\ \mathbf{V}_{2j} & \hat{\mathbf{V}}_{1\bar{j}} & c_{3\bar{j}}\mathbf{I} \end{pmatrix}. \tag{25}$$

Matrices $\mathbf{V}_{ij}$ will be referred to as *V matrices*, $\mathbf{V}_j$ as *large V matrices*.

Additional extremely useful properties of V matrices can be obtained from Eq. (23). This system is redundant in comparison to the system Eq. (14) from which it has been derived. So, if one of the subsystems in Eq. (23) holds, then the other subsystems hold automatically because of the following relations that can be derived from the definitions [Eqs. (12), (13), (16), (24), and characteristic equation Eq. (15)]:

$$|\mathbf{V}_{ij}| = c_{\bar{i}j}c_{\bar{i}j}, \qquad \mathbf{V}_{\bar{i}j}\mathbf{V}_{\bar{i}j} = c_{ij}\hat{\mathbf{V}}_{ij}. \tag{26}$$

From the same set of equations, the following relation can be derived as well:

$$\hat{\mathbf{V}}_j\mathbf{V}_j = \mathrm{diag}\left(c_{1j}p_j\mathbf{I},\ c_{2\bar{j}}p_{\bar{j}}\mathbf{I},\ c_{3\bar{j}}p_{\bar{j}}\mathbf{I}\right), \tag{27}$$

where p_j are the first derivatives of the polynomial $\hat{P}(\hat{\lambda})$ [Eq. (18)] at $\hat{\lambda} = \hat{\lambda}_j$. They can be expressed via $\overleftrightarrow{\mathbf{M}}$ eigenvalues using Viète's theorem [16]:

$$\begin{aligned} p_j &= \hat{P}'(\hat{\lambda}_j) = 3\hat{\lambda}_j^2 + 2B\hat{\lambda}_j + C \\ &= 3\hat{\lambda}_j^2 - 2(\hat{\lambda}_j + \hat{\lambda}_{\bar{j}} + \hat{\lambda}_{\bar{j}})\hat{\lambda}_j + (\hat{\lambda}_{\bar{j}}\hat{\lambda}_{\bar{j}} + \hat{\lambda}_{\bar{j}}\hat{\lambda}_j + \hat{\lambda}_j\hat{\lambda}_{\bar{j}}) \\ &= (\hat{\lambda}_{\bar{j}} - \hat{\lambda}_j)(\hat{\lambda}_{\bar{j}} - \hat{\lambda}_j). \end{aligned} \tag{28}$$

VI. EIGENVECTOR NORMALIZATION

V matrices consist of the recurrent matrix eigenvectors. To make them directly applicable to the further transport matrix transformations toward the desired block-diagonal form, a normalization procedure should be chosen. The proposal here is to divide each eigenvector corresponding to the $\hat{\lambda}_j$ by p_j. On the one hand, this excludes all degenerated cases from the scope, because if one of the eigenvalues is degenerated more than twice, then there are zero values among p_j, according to Eq. (28). However, it is shown in Appendix B that the approach proposed here is, in general, not applicable to degenerated cases. It is still to be extended to include them. On the other hand, this normalization procedure allows us to describe the coupling between degrees of freedom in the same way as in the well-known Lebedev-Bogacz parameterization [3]. It is shown in Sec. XI after reduction to the 4×4 case. Moreover, eigenvector matrices normalized in such a way have a number of useful properties.

According to Eq. (25), normalized matrices can be written as follows:

$$\mathbf{W}_j = \begin{pmatrix} u_{1j}\mathbf{I} & \mathbf{W}_{3\bar{j}} & \hat{\mathbf{W}}_{2\bar{j}} \\ \hat{\mathbf{W}}_{3j} & u_{2\bar{j}}\mathbf{I} & \mathbf{W}_{1\bar{j}} \\ \mathbf{W}_{2j} & \hat{\mathbf{W}}_{1\bar{j}} & u_{3\bar{j}}\mathbf{I} \end{pmatrix}, \tag{29}$$

where

$$\mathbf{W}_{ij} = \frac{\mathbf{V}_{ij}}{p_j}, \qquad u_{ij} = \frac{c_{ij}}{p_j}. \tag{30}$$

$\mathbf{W}_{ij}$ matrices will be referred to as *W matrices*, $\mathbf{W}_j$ as *large W matrices*. $\mathbf{W}_{ij}$ and u_{ij} have properties similar to Eq. (26):

$$|\mathbf{W}_{ij}| = u_{\bar{i}j}u_{\bar{i}j}, \qquad \mathbf{W}_{\bar{i}j}\mathbf{W}_{\bar{i}j} = u_{ij}\hat{\mathbf{W}}_{ij}, \tag{31}$$

which can be also expressed as

$$\begin{aligned}\mathbf{W}_{1j}\mathbf{W}_{2j}\mathbf{W}_{3j} &= \mathbf{W}_{2j}\mathbf{W}_{3j}\mathbf{W}_{1j} \\ &= \mathbf{W}_{3j}\mathbf{W}_{1j}\mathbf{W}_{2j} = u_{1j}u_{2j}u_{3j}\mathbf{I}.\end{aligned} \tag{32}$$

In Appendix C, additional relations between W matrices are shown, which have not been used directly in other parts of the paper.

The following useful equality for $\mathbf{W}_j$ can be obtained from Eqs. (12), (13), (15), (16), (29), and (30):

$$\mathbf{W}_1 + \mathbf{W}_2 + \mathbf{W}_3 = \mathbf{I}_6. \tag{33}$$

Additional $\mathbf{W}_{ij}$ and u_{ij} properties can be derived from it:

$$\mathbf{W}_{i1} + \mathbf{W}_{i2} + \mathbf{W}_{i3} = \mathbf{0}, \tag{34}$$

$$\begin{aligned}u_{i1} + u_{i2} + u_{i3} &= 1 \\ u_{1j} + u_{2j} + u_{3j} &= 1\end{aligned}, \tag{35}$$

therefore, the following equality similar to Eq. (27) holds:

$$\hat{\mathbf{W}}_j\mathbf{W}_j = \mathbf{U}_j, \tag{36}$$

where

$$\mathbf{U}_j = \mathrm{diag}(u_{1j}\mathbf{I},\, u_{2\bar{j}}\mathbf{I},\, u_{3\bar{j}}\mathbf{I}). \tag{37}$$

u_{ij} describes the coupling between different degrees of freedom, a matrix $\mathbf{U}$ formed of them will be referred to as *coupling matrix*:

$$\mathbf{U} = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{pmatrix}. \tag{38}$$

According to Eq. (35), it has only four independent elements. In the most common case of a fully uncoupled motion, it is a unity matrix. Then the best option is to take the diagonal elements u_{11}, u_{22}, u_{33} as three independent parameters. The simplest way to define the fourth and keep the notation symmetric with respect to all indices is the following:

$$l = u_{32} - u_{23} = u_{13} - u_{31} = u_{21} - u_{12}, \tag{39}$$

these relations hold due to Eq. (35). According to the definition, parameter l will be referred to as *coupling asymmetry* because it is related to the asymmetry of the coupling matrix. Thus, all off-diagonal elements of the coupling matrix can be expressed as follows:

$$\begin{aligned}u_{i\bar{i}} &= \frac{1}{2}(1 - l - u_{ii} - u_{\bar{i}\bar{i}} + u_{\bar{i}i}), \\ u_{i\bar{i}} &= \frac{1}{2}(1 + l - u_{ii} - u_{\bar{i}i} + u_{i\bar{i}}).\end{aligned} \tag{40}$$

According to Eq. (35), coupling matrix has at least one nonzero element in each row and column. The number of rows and columns containing more than one nonzero element is equal and defines the coupling type: 3 for a fully coupled case, 2 for a partly coupled case (1 of 3 degrees of freedom is uncoupled), and 0 for a noncoupled case. In the noncoupled case, all $\mathbf{W}_{ij} = \mathbf{0}$, in the partly coupled case (if the kth degree of freedom is uncoupled), only $\mathbf{W}_{k\bar{k}}$ and $\mathbf{W}_{\bar{k}k}$ are nonzero and $|\mathbf{W}_{k\bar{k}}|, |\mathbf{W}_{\bar{k}k}| \neq 0$.

VII. TWISS PARAMETERIZATION

Now everything has been prepared for transforming $\mathbf{M}$ into the block-diagonal form and introducing Twiss parameterization for the resulting blocks.

One can go back to Eq. (7) and notice that $\overleftrightarrow{\mathbf{M}}$ eigenvectors corresponding to the $\hat{\lambda}$ eigenvalue form a two-dimensional space with the basis of $\mathbf{M}$ eigenvectors corresponding to λ_1 and λ_2 (degenerated cases are excluded from the scope). Therefore, the following 2×2 $\mathbf{Q}_{ij}$ matrices may be found:

$$\mathbf{M}\mathbf{W}_j = \mathbf{W}_j\mathbf{Q}_j, \tag{41}$$

where

$$\mathbf{Q}_j = \mathrm{diag}(\mathbf{Q}_{1j},\, \mathbf{Q}_{2\bar{j}},\, \mathbf{Q}_{3\bar{j}}).$$

The $\mathbf{Q}_{ij}$ determinants can be obtained by multiplying each side of Eq. (41) by its symplectic conjugate:

$$\hat{\mathbf{W}}_j\hat{\mathbf{M}}\mathbf{M}\mathbf{W}_j = \hat{\mathbf{Q}}_j\hat{\mathbf{W}}_j\mathbf{W}_j\mathbf{Q}_j.$$

Then, according to Eqs. (5) and (36),

$$|\mathbf{Q}_{ij}| = 1, \quad \text{if } u_{ij} \neq 0. \tag{42}$$

Large Twiss matrices $\mathbf{T}_j$ will be defined as follows:

$$\mathbf{T}_j = \hat{\mathbf{W}}_j\mathbf{M}\mathbf{W}_j. \tag{43}$$

According to Eqs. (36) and (41), they are block diagonal:

$$\mathbf{T}_j = \mathrm{diag}(\mathbf{T}_{1j},\, \mathbf{T}_{2\bar{j}},\, \mathbf{T}_{3\bar{j}}),$$

where $\mathbf{T}_{ij}$ will be referred to as *Twiss matrices*, they are related to $\mathbf{Q}_{ij}$:

$$\mathbf{T}_{ij} = u_{ij}\mathbf{Q}_{ij}, \tag{44}$$

this equation can be regarded as $\mathbf{Q}_{ij}$ definition. Therefore, Eq. (43) describes the desired transport matrix transformation to the block-diagonal form.

According to Eq. (33),

$$\mathbf{T}_j = \mathbf{M}\mathbf{W}_j - \hat{\mathbf{W}}_{\bar{j}}\mathbf{M}\mathbf{W}_j - \hat{\mathbf{W}}_{\bar{j}}\mathbf{M}\mathbf{W}_j.$$

Here the diagonal blocks of the last two terms are zeros, therefore $\mathbf{T}_{ij}$ can be easily expressed via $\mathbf{M}_{ij}$ and $\mathbf{W}_{ij}$, without the calculation of the triple matrix products in Eq. (43):

$$\mathbf{T}_{ij} = u_{ij}\mathbf{M}_{ii} + \mathbf{M}_{i\bar{i}}\hat{\mathbf{W}}_{\bar{i}j} + \mathbf{M}_{i\bar{i}}\mathbf{W}_{\bar{i}j}. \tag{45}$$

$\mathbf{T}_{ij}$ determinants can be found directly from Eqs. (42) and (44). To obtain their traces, one should add Eq. (43) to its symplectic conjugate:

$$\mathrm{diag}((\mathrm{Tr}\,\mathbf{T}_{1j})\mathbf{I}, (\mathrm{Tr}\,\mathbf{T}_{2\bar{j}})\mathbf{I}, (\mathrm{Tr}\,\mathbf{T}_{3\bar{j}})\mathbf{I}) = \hat{\mathbf{W}}_j\overleftrightarrow{\mathbf{M}}\mathbf{W}_j.$$

Finally,

$$\begin{aligned} |\mathbf{T}_{ij}| &= u_{ij}^2 \\ \mathrm{Tr}\,\mathbf{T}_{ij} &= u_{ij}\hat{\lambda}_j \end{aligned}. \tag{46}$$

Then each $\mathbf{T}_{ij}$ can be parameterized with two real parameters α_{ij} and β_{ij}, similarly to the well-known Twiss parameterization [2]:

$$\begin{aligned} \boldsymbol{T}_{ij} &= \begin{pmatrix} u_{ij}\cos\mu_j + \alpha_{ij}\sin\mu_j & \beta_{ij}\sin\mu_j \\ -\gamma_{ij}\sin\mu_j & u_{ij}\cos\mu_j - \alpha_{ij}\sin\mu_j \end{pmatrix}, \\ &\text{where } \beta_{ij}\gamma_{ij} = u_{ij}^2 + \alpha_{ij}^2, \quad \mu_j = \pm\arg\lambda_j. \end{aligned} \tag{47}$$

This can be rewritten as

$$\begin{aligned} \mathbf{T}_{ij} &= \mathbf{I}u_{ij}\cos\mu_j + \mathbf{J}_{ij}\sin\mu_j, \\ \text{where } \mathbf{J}_{ij} &= \begin{pmatrix} \alpha_{ij} & \beta_{ij} \\ -\gamma_{ij} & -\alpha_{ij} \end{pmatrix}. \end{aligned} \tag{48}$$

An apparent ambiguity should be noted here: $\mathbf{T}_{ij}$ does not change if the signs of α_{ij}, β_{ij}, and μ_j are flipped simultaneously. The way to avoid this has been proposed already by Courant and Snyder in [2]. In case of non-coupled motion, phase advance signs are chosen to make β functions non-negative. To keep this convention in the coupled case, one should choose "diagonal" β functions β_{jj} to be non-negative, which defines the signs of μ_j unambiguously. Thus, the signs of $\beta_{\bar{j}j}$ and $\beta_{\bar{j}\bar{j}}$ are defined as well, and they are not necessarily non-negative. Finally,

$$\begin{aligned} \mu_j &= \mathrm{sgn}\,(\mathbf{T}_{jj})_{12}|\cos^{-1}(\hat{\lambda}_j/2)|, \\ \alpha_{ij} &= \frac{(\mathbf{T}_{ij})_{11} - (\mathbf{T}_{ij})_{22}}{2\sin\mu_j}, \\ \beta_{ij} &= \frac{(\mathbf{T}_{ij})_{12}}{\sin\mu_j}. \end{aligned}$$

VIII. TRANSPORT MATRIX RESTORING

To make the parameterization ready-to-use, not only direct but also inverse procedure should be described in detail. One should begin with restoring the coupling matrix $\mathbf{U}$ from u_{ii} and l using Eq. (40), and then restoring $\mathbf{T}_{ij}$ and $\mathbf{T}_j$ from α_{ij}, β_{ij}, u_{ij}, and μ_j using Eq. (47).

W matrices can be expressed through other parameters. The first step in this direction is to obtain their commutation rules with $\mathbf{Q}_{ij}$ and $\mathbf{J}_{ij}$. Using Eqs. (29) and (31), large W matrices can be expressed through each other:

$$\mathbf{W}_j\begin{pmatrix} u_{3j}\mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & u_{1\bar{j}}\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & u_{2\bar{j}}\mathbf{I} \end{pmatrix} = \mathbf{W}_{\bar{j}}\begin{pmatrix} \mathbf{0} & \mathbf{W}_{3\bar{j}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{W}_{1\bar{j}} \\ \mathbf{W}_{2j} & \mathbf{0} & \mathbf{0} \end{pmatrix}. \tag{49}$$

Using this relation, one can exclude $\mathbf{M}$ from Eq. (41):

$$\begin{aligned} &\mathbf{W}_{\bar{j}}\mathbf{Q}_{\bar{j}}\begin{pmatrix} \mathbf{0} & \mathbf{W}_{3\bar{j}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{W}_{1\bar{j}} \\ \mathbf{W}_{2j} & \mathbf{0} & \mathbf{0} \end{pmatrix} \\ &= \mathbf{W}_{\bar{j}}\begin{pmatrix} \mathbf{0} & \mathbf{W}_{3\bar{j}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{W}_{1\bar{j}} \\ \mathbf{W}_{2j} & \mathbf{0} & \mathbf{0} \end{pmatrix}\mathbf{Q}_j. \end{aligned}$$

Here $\mathbf{W}_{\bar{j}}$ can be canceled on both sides without loss of generality, then

$$\mathbf{W}_{ij}\mathbf{Q}_{\bar{i}j} = \mathbf{Q}_{\bar{i}j}\mathbf{W}_{ij}, \tag{50}$$

which can be rewritten as

$$\mathbf{W}_{ij}u_{\bar{i}j}\mathbf{J}_{\bar{i}j} = u_{\bar{i}j}\mathbf{J}_{\bar{i}j}\mathbf{W}_{ij}. \tag{51}$$

Such equations will be referred to as 2×2 *commutation matrix equations*. Their general solution is given in Appendix D. An important detail here is that all $\mathbf{J}_{ij}$ matrices are traceless, i.e., $\mathrm{Tr}\,\mathbf{J}_{ij} = 0$.

Combining these commutation rules with Eqs. (31) and (34), one obtains the following equation system:

$$\begin{aligned}
&\mathbf{W}_{i\bar{j}} u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} = u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{W}_{i\bar{j}} \\
&\mathbf{W}_{\bar{i}j} u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} = u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{W}_{\bar{i}j} \\
&\mathbf{W}_{ij} u_{\bar{i}j} \mathbf{J}_{\bar{i}j} = u_{\bar{i}j} \mathbf{J}_{\bar{i}j} \mathbf{W}_{ij} \\
&\mathbf{W}_{ij} + \mathbf{W}_{i\bar{j}} + \mathbf{W}_{\bar{i}j} = \mathbf{0} \\
&|\mathbf{W}_{ij}| = u_{\bar{i}j} u_{\bar{i}j} \\
&|\mathbf{W}_{i\bar{j}}| = u_{\bar{i}\bar{j}} u_{\bar{i}\bar{j}} \\
&|\mathbf{W}_{\bar{i}j}| = u_{\bar{i}\bar{j}} u_{\bar{i}\bar{j}}
\end{aligned} . \tag{52}$$

Since the determinants of $\mathbf{J}_{ij}$ are known from Eq. (47), this system is similar to Eq. (E1) in Appendix E. General solution is explained there in detail using a simplified notation. Here only the most important outcomes are given.

First, two of the W matrices in Eq. (52) can be expressed through the third one:

$$\begin{aligned}
&\tau_{ij} \mathbf{W}_{i\bar{j}} = \mathbf{A} u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} + u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{A}, \\
&\quad \text{where } \mathbf{A} = u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{W}_{ij} - u_{\bar{i}\bar{j}} \mathbf{W}_{ij} \mathbf{J}_{\bar{i}\bar{j}}, \\
&\tau_{ij} \mathbf{W}_{\bar{i}j} = \mathbf{B} u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} + u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{B}, \\
&\quad \text{where } \mathbf{B} = u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{W}_{ij} - u_{\bar{i}\bar{j}} \mathbf{W}_{ij} \mathbf{J}_{\bar{i}\bar{j}},
\end{aligned} \tag{53}$$

where

$$\tau_{ij} = \mathrm{Tr}\,(u_{\bar{i}\bar{j}} u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} - u_{\bar{i}\bar{j}} u_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}} \mathbf{J}_{\bar{i}\bar{j}}).$$

If for a given i, all $\tau_{ij} = 0$, then Eq. (52) has an infinite set of solutions and the approach proposed in Appendix E cannot be applied. On the one hand, it is still an open question if this situation can be realized in the fully coupled case. This would indicate a *special point of the Twiss parameterization*, a point where the transport matrix cannot be restored from the parameters. Their presence is not detrimental for the entire Twiss parameterization concept as long as one can detect them during the parameterization process.

On the other hand, in the partly coupled and noncoupled cases, all $\tau_{ij} = 0$, and this does not indicate a special point. Then two options are possible: (i) $|\mathbf{W}_{ij}| = |\mathbf{W}_{i\bar{j}}| = |\mathbf{W}_{\bar{i}\bar{j}}| = 0$, then there is the only solution $\mathbf{W}_{ij} = \mathbf{W}_{i\bar{j}} = \mathbf{W}_{\bar{i}\bar{j}} = \mathbf{0}$. (ii) $\exists k : |\mathbf{W}_{i\bar{k}}| = |\mathbf{W}_{\bar{i}k}| \neq 0$, then $\mathbf{W}_{ik} = \mathbf{0}$, $\mathbf{W}_{i\bar{k}} = -\mathbf{W}_{\bar{i}k}$. Then the system Eq. (52) is reduced to the one described in Appendix F and has two solutions that differ only in signs.

To restore all W matrices, the system Eq. (52) should be solved for three different i values. As it was explained at the end of Sec. VI, in the noncoupled case, the former option realizes thrice, therefore only one valid set of W matrices exists. In the partly coupled case, the former option realizes twice and the latter once, which results in two valid sets of W matrices.

In the fully coupled case, all options for Eq. (52) solution set should be considered, which may consist of 0, 1, 2, 4, and infinite number of solutions. The latter case would correspond to a special point. In simulations performed for fully coupled lattices, only the option with four solutions was realized. This means that there are $4^3 = 64$ valid combinations of W matrices. At the same time, W matrices should satisfy Eq. (32). In simulations, this was the case only for four of these combinations. Among these four, the only difference within each pair is a simultaneous sign flip of 6 $\mathbf{W}_{ij}$ for two of three possible i values. Here it becomes obvious that the partly coupled and noncoupled cases are subsets of the general fully coupled case, number of solutions is reduced due to zeroing out part of (or all) W matrices.

Once all elements of the coupling matrix and W matrices have been found, one can write down $\mathbf{W}_j$ [see Eq. (29)] and $\mathbf{U}_j$ [see Eq. (37)]. According to W matrices properties, if $\mathbf{U}_j^{-1}$ exists, then

$$\mathbf{W}_j \mathbf{U}_j^{-1} \hat{\mathbf{W}}_j = \mathbf{I}_6. \tag{54}$$

Therefore, it follows from Eq. (43) that

$$\mathbf{M} = \mathbf{W}_j \mathbf{U}_j^{-1} \mathbf{T}_j \mathbf{U}_j^{-1} \hat{\mathbf{W}}_j. \tag{55}$$

Here index j can take any value for which $\mathbf{U}_j^{-1}$ exists. Therefore, it should be chosen as follows to increase accuracy:

$$j = \begin{cases} 1, & \min_i |u_{ii}| \geq \min_i |u_{i\bar{i}}|, \min_i |u_{\bar{i}\bar{i}}|, \\ 2, & \min_i |u_{i\bar{i}}| \geq \min_i |u_{\bar{i}\bar{i}}|, \min_i |u_{ii}|, \\ 3, & \min_i |u_{\bar{i}\bar{i}}| \geq \min_i |u_{ii}|, \min_i |u_{i\bar{i}}|. \end{cases}$$

Theoretically, it is possible to construct a coupling matrix for which the conditions Eq. (35) are fulfilled but all three $\mathbf{U}_j^{-1}$ do not exist.[4] This would indicate a special point, however, such a case has never realized in simulations.

Noting that there are four possible combinations of W matrices, Eq. (55) gives four options for the transport matrix $\mathbf{M}$ restored from parameters:

$$\{\mathbf{M},\ \mathbf{F}_1 \mathbf{M} \mathbf{F}_1^{-1},\ \mathbf{F}_2 \mathbf{M} \mathbf{F}_2^{-1},\ \mathbf{F}_3 \mathbf{M} \mathbf{F}_3^{-1}\}, \tag{56}$$

[4] An example of such a coupling matrix:

$$\mathbf{U} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

where

$$\begin{aligned}\mathbf{F}_1 &= \mathrm{diag}(-\mathbf{I}, \mathbf{I}, \mathbf{I})\\ \mathbf{F}_2 &= \mathrm{diag}(\mathbf{I}, -\mathbf{I}, \mathbf{I})\,.\\ \mathbf{F}_3 &= \mathrm{diag}(\mathbf{I}, \mathbf{I}, -\mathbf{I})\end{aligned} \tag{57}$$

Matrices $\mathbf{F}_j$ will be referred to as *sign flippers*, each of them performs a sign flip of one pair of accelerator coordinates (either x, x', or y, y', or z, z'). $\mathbf{F}_j$ are symplectic, therefore, sign flippers may be regarded as fictitious beamline elements. The physical meaning that can be ascribed to them will be explained in the next section.

The set of the four options for the restored transport matrix is defined by 25 parameters: nine α_{ij}, nine β_{ij}, three u_{ii}, one l for each point, and three μ_j for the entire lattice. A symplectic 6×6 matrix has only 21 independent element, thus there are four equalities connecting the parameters at each point. Three of them are contained in Eq. (32), which have been used for the selection of the valid W-matrix options. A closed expression for the last one is still to be found.[5]

The method to choose the correct option out of these four is not so obvious. In [3], for a 4×4 transport matrix, two parameters ν_1 and ν_2 have been introduced, one per an off-diagonal 2×2 block. To keep the same efficiency, for a 6×6 matrix, six additional parameters could be introduced. However, it is still to be found how to do this in a symmetric way. As an intermediate solution, all W matrices (36 elements in total) can be included into the parameter set. On the one hand, this increases significantly the number of parameters. On the other hand, it allows us to skip the most computationally intensive part of the transport matrix restoring procedure.

IX. BETATRON PHASE ADVANCES

As it was already established in the introduction, $\mathbf{M}$ is a transport matrix of a period in a periodic lattice. Although it depends on the azimuth which has been taken as a border between adjacent periods, this dependency becomes important only in this section. It is possible to write down transport matrix $\mathbf{M}(s)$ as a function of azimuth s. If the matrix $\mathbf{M}^{(1\to 2)}$ describes transport from azimuth s_1 to s_2, then (see e.g., [1]),

$$\mathbf{M}(s_2) = \mathbf{M}^{(1\to 2)}\mathbf{M}(s_1)(\mathbf{M}^{(1\to 2)})^{-1}. \tag{58}$$

A valid parameterization must allow unambiguous restoring of $\mathbf{M}(s)$ at each point along the lattice, and transport matrices between each pair of them from parameter values at these points. One may expect that at least for 2×2 matrices, Twiss parameters α and β at each point and $\mathbf{M}(s)$ eigenvalues (which do not depend on s) are enough for this purpose. However, this is not the case. It is enough to restore $\mathbf{M}(s)$, but transport matrices between any two points can be restored only up to the sign because of Eq. (58). This means that inserting $-\mathbf{I}$ coordinate transformations at arbitrary positions, one does not change $\mathbf{M}(s)$.

This ambiguity can be solved by introducing *betatron phase advances*. The corresponding formulas for the 2×2 case (or uncoupled optics) are given e.g., in [1]. In the coupled case, betatron phase advances can be introduced for the block-diagonal large Twiss matrices. Let superscripts $^{(1)}$ and $^{(2)}$ applied to $\mathbf{W}_j$, $\mathbf{T}_j$, $\mathbf{U}_j$ matrices and their elements denote their values at points s_1 and s_2, respectively. Matrices $\mathbf{N}_j^{(1\to 2)}$ can be defined in the following way:

$$\mathbf{N}_j^{(1\to 2)} = \hat{\mathbf{W}}_j^{(2)}\mathbf{M}^{(1\to 2)}\mathbf{W}_j^{(1)}. \tag{59}$$

Then using Eqs. (36), (54), (55), (58), and (59), one can find the relation between $\mathbf{T}_j^{(1)}$ and $\mathbf{T}_j^{(2)}$:

$$\mathbf{T}_j^{(2)} = \mathbf{N}_j^{(1\to 2)}\left(\mathbf{U}_j^{(1)}\right)^{-1}\mathbf{T}_j^{(1)}\left(\mathbf{U}_j^{(1)}\right)^{-1}\left(\mathbf{N}_j^{(1\to 2)}\right)^{-1}. \tag{60}$$

$\mathbf{N}_j^{(1\to 2)}$ are block diagonal because $\mathbf{T}_j$ describe orthogonal modes:

$$\mathbf{N}_j^{(1\to 2)} = \mathrm{diag}\left(\mathbf{N}_{1\vec{j}}^{(1\to 2)}, \mathbf{N}_{2\vec{j}}^{(1\to 2)}, \mathbf{N}_{3\vec{j}}^{(1\to 2)}\right),$$

therefore, $(\mathbf{U}_j^{(1)})^{-1}$ factors from Eq. (60) are canceled in the phase advance $\Delta\psi_{ij}^{(1\to 2)}$ definition:

$$\begin{aligned}\Delta\psi_{ij}^{(1\to 2)} = &\tan^{-1}\frac{u_{ij}^{(1)}(\mathbf{N}_{ij}^{(1\to 2)})_{12}}{\beta_{ij}^{(1)}(\mathbf{N}_{ij}^{(1\to 2)})_{11} - \alpha_{ij}^{(1)}(\mathbf{N}_{ij}^{(1\to 2)})_{12}}\\ &+ \pi[1-\theta(\mathrm{Tr}\,\mathbf{N}_{ij}^{(1\to 2)})],\end{aligned} \tag{61}$$

where $\theta(x)$ is the Heaviside function (defined as 1 at $x=0$), $\alpha_{ij}^{(1)}$, $\beta_{ij}^{(1)}$, and $u_{ij}^{(1)}$ are Twiss parameters and coupling matrix elements at s_1.

This brings us back to the sign-flipper concept introduced in the previous section [see Eq. (57)]. Sign flippers may be regarded as *phase trombones*, fictitious thin beamline elements keeping α and β Twiss parameters and changing only the betatron phase advances. In this case, $\mathbf{F}_i$ changes three phase advances $\Delta\psi_{ij}^{(1\to 2)}$ by π.

X. BEAM SIZES AND EMITTANCES

After setting up the direct and inverse parameterization procedure for the fully coupled case, the emittance concept

[5]It should be symmetric with respect to all indices and most probably related to Eq. (C2) in Appendix C because they are the only relations between W matrices explicitly including l, which is index independent.

should be updated as well. According to the definition, $\bar{\boldsymbol{\Xi}}$ is a coordinate column vector of a particle. Let $\tilde{\bar{\boldsymbol{\Xi}}}_j$ be the same vector expressed in the basis of $\mathbf{W}_j$ columns, then

$$\bar{\boldsymbol{\Xi}} = \mathbf{W}_j \tilde{\bar{\boldsymbol{\Xi}}}_j. \tag{62}$$

Particles of the beam have a certain distribution over all six coordinates that can be characterized with the second-order moments matrices $\boldsymbol{\Sigma}$ and $\tilde{\boldsymbol{\Sigma}}$ in these bases, respectively:

$$\begin{aligned} \boldsymbol{\Sigma} &= \langle \bar{\boldsymbol{\Xi}} \bar{\boldsymbol{\Xi}}^T \rangle \\ \tilde{\boldsymbol{\Sigma}}_j &= \langle \tilde{\bar{\boldsymbol{\Xi}}}_j \tilde{\bar{\boldsymbol{\Xi}}}_j^T \rangle \end{aligned}, \tag{63}$$

where angle brackets mean averaging over the particles of the beam. From Eq. (62), one can easily obtain the relation between $\boldsymbol{\Sigma}$ and $\tilde{\boldsymbol{\Sigma}}_j$:

$$\boldsymbol{\Sigma} = \mathbf{W}_j \tilde{\boldsymbol{\Sigma}}_j \mathbf{W}_j^T. \tag{64}$$

Let $\mathbf{M}$, as usual, be transport matrix of a period in a periodic lattice. The beam is referred to as *matched with the lattice* if $\boldsymbol{\Sigma}$ is preserved after an arbitrary integer number of periods:

$$\boldsymbol{\Sigma} = \langle \mathbf{M}\bar{\boldsymbol{\Xi}} (\mathbf{M}\bar{\boldsymbol{\Xi}})^T \rangle = \mathbf{M}\boldsymbol{\Sigma}\mathbf{M}^T. \tag{65}$$

Substituting Eqs. (36), (43), and (64) into Eq. (65) one obtains

$$\mathbf{U}_j \tilde{\boldsymbol{\Sigma}}_j \mathbf{U}_j = \mathbf{T}_j \tilde{\boldsymbol{\Sigma}}_j \mathbf{T}_j^T. \tag{66}$$

This equation can be transformed into a 2×2 commutation matrix equation of the form $\mathbf{XA} = \mathbf{BX}$ (see Appendix D). If $|\mathbf{A}| = |\mathbf{B}| \neq 0$, then it has a nontrivial solution only in the case of $\operatorname{Tr}\mathbf{A} = \operatorname{Tr}\mathbf{B}$. Therefore, $\tilde{\boldsymbol{\Sigma}}_j$ are block diagonal because of Eq. (46) and can be defined as follows:

$$\tilde{\boldsymbol{\Sigma}}_j = \operatorname{diag}(\tilde{\boldsymbol{\Sigma}}_{1j}, \tilde{\boldsymbol{\Sigma}}_{2\bar{j}}, \tilde{\boldsymbol{\Sigma}}_{3\bar{j}}),$$

where $\tilde{\boldsymbol{\Sigma}}_{ij}$ are 2×2 matrices. Thus, Eq. (66) contains only block-diagonal matrices, therefore, to obtain $\tilde{\boldsymbol{\Sigma}}_{ij}$, one should rewrite Eq. (65) for 2×2 matrices $\tilde{\boldsymbol{\Sigma}}$ and $\tilde{\mathbf{M}}$:

$$\tilde{\boldsymbol{\Sigma}} = \tilde{\mathbf{M}} \tilde{\boldsymbol{\Sigma}} \tilde{\mathbf{M}}^T,$$

where $\tilde{\boldsymbol{\Sigma}} = \tilde{\boldsymbol{\Sigma}}^T$ and $|\tilde{\mathbf{M}}| = 1$. This equation has the following solution:

$$\tilde{\boldsymbol{\Sigma}} = k \begin{pmatrix} \tilde{m}_{12} & \dfrac{\tilde{m}_{22} - \tilde{m}_{11}}{2} \\ \dfrac{\tilde{m}_{22} - \tilde{m}_{11}}{2} & -\tilde{m}_{21} \end{pmatrix}, \tag{67}$$

where $\tilde{m}_{ij}$ are $\tilde{\mathbf{M}}$ elements and k is an arbitrary coefficient.

If $\tilde{\mathbf{M}}$ is a transport matrix in the 2×2 case, then *rms emittance,* ε_{rms}, of the beam is defined as follows [1]:

$$\varepsilon_{\text{rms}} = \sqrt{\langle x^2 \rangle \langle x'^2 \rangle - \langle x x' \rangle^2} = \sqrt{|\tilde{\boldsymbol{\Sigma}}|}. \tag{68}$$

If one introduces Twiss parameterization for $\tilde{\mathbf{M}}$ with the Twiss parameters $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ [combined into a 2×2 matrix $\tilde{\mathbf{J}}$, according to Eq. (48)] and $\tilde{\mu}$, then

$$\tilde{\mathbf{M}} = \mathbf{I} \cos\tilde{\mu} + \tilde{\mathbf{J}} \sin\tilde{\mu}$$

and

$$\tilde{\boldsymbol{\Sigma}} = \varepsilon_{\text{rms}} \begin{pmatrix} \tilde{\beta} & -\tilde{\alpha} \\ -\tilde{\alpha} & \tilde{\gamma} \end{pmatrix} = -\varepsilon_{\text{rms}} \tilde{\mathbf{J}} \mathbf{S}. \tag{69}$$

Therefore, $\tilde{\boldsymbol{\Sigma}}_j$ can be found in the following form:

$$\tilde{\boldsymbol{\Sigma}}_j = -\operatorname{diag}(\varepsilon_{1j} \mathbf{J}_{1j} \mathbf{S}, \varepsilon_{2\bar{j}} \mathbf{J}_{2\bar{j}} \mathbf{S}, \varepsilon_{3\bar{j}} \mathbf{J}_{3\bar{j}} \mathbf{S}),$$

where ε_{ij} are free parameters. Using Eqs. (49) and (65), those of them with corresponding $u_{ij} \neq 0$ can be expressed through each other:

$$\varepsilon_{1j} u_{1j}^2 = \varepsilon_{2j} u_{2j}^2 = \varepsilon_{3j} u_{3j}^2 = \varepsilon_j,$$

where ε_j are *emittances*. They are the only three independent parameters in the second-order moments matrix $\boldsymbol{\Sigma}$ matched with a periodic lattice with 6×6 transport matrix $\mathbf{M}$. So, if $u_{ii} \neq 0$, then $\boldsymbol{\Sigma}$ can be found as follows:

$$\boldsymbol{\Sigma} = -\mathbf{W}_1 \operatorname{diag}\left(\frac{\varepsilon_1}{u_{11}^2} \mathbf{J}_{11}, \frac{\varepsilon_2}{u_{22}^2} \mathbf{J}_{22}, \frac{\varepsilon_3}{u_{33}^2} \mathbf{J}_{33} \right) \mathbf{S} \mathbf{W}_1^T.$$

XI. 4 × 4 TRANSPORT MATRIX

At this point, the development of the symmetric Twiss parameterization of a 6×6 symplectic transport matrix is completed, as well as the inverse procedure and the emittance concept. In the present section, it will be reduced to the 4×4 case and checked against the well-known Lebedev-Bogacz parameterization [3].

To perform such a reduction, one should take e.g., $\mathbf{M}_{13} = \mathbf{M}_{31} = \mathbf{M}_{23} = \mathbf{M}_{32} \equiv \mathbf{0}$ in Eq. (6). This leads to $\mathbf{R}_1 = \mathbf{R}_2 = \mathbf{0}$ and $a_{33} = 0$. Then it can be derived that $u_{13} = u_{31} = u_{23} = u_{32} \equiv 0$ and only $\mathbf{W}_{31}$ and $\mathbf{W}_{32}$ are nonzero among W matrices. This corresponds to the case when the horizontal and vertical dynamics is coupled, but the longitudinal one is independent. From now on, we can exclude the longitudinal degree of freedom completely and switch to 4×4 matrices, which allows significant simplification of the notation.

A 4×4 transport matrix can be written in a block form:

$$\mathbf{M}=\begin{pmatrix}\mathbf{M}_{11} & \mathbf{M}_{12}\\ \mathbf{M}_{21} & \mathbf{M}_{22}\end{pmatrix}.$$

Then the recurrent matrix can be rewritten as follows:

$$\overleftrightarrow{\mathbf{M}}=\begin{pmatrix}b_1\mathbf{I} & \mathbf{R}\\ \hat{\mathbf{R}} & b_2\mathbf{I}\end{pmatrix},$$

where

$$\mathbf{R}=\mathbf{M}_{12}+\hat{\mathbf{M}}_{21}.$$

a_{ij} definition is the same as in Eq. (13), characteristic equation has the following form:

$$a_{1j}a_{2j}-d=0,$$

where

$$d=|\mathbf{R}|.$$

Therefore, $\overleftrightarrow{\mathbf{M}}$ eigenvalues are:

$$\hat{\lambda}_{1,2}=\frac{1}{2}\left(b_1+b_2\pm\sqrt{(b_1-b_2)^2+4d}\right).$$

The same definitions for c_{ij}, $\mathbf{V}_{ij}$, and p_j could be used as in the 6×6 case, but they are not necessary, one may proceed directly to the coupling matrix and W matrices concept. Coupling matrix contains only one independent parameter and can be expressed as follows:

$$\mathbf{U}=\begin{pmatrix}1-u & u\\ u & 1-u\end{pmatrix},$$

where

$$u=\frac{a_{11}}{\delta}=-\frac{a_{22}}{\delta},\qquad \delta=\hat{\lambda}_2-\hat{\lambda}_1.$$

Parameter u will be referred to as *coupling parameter*, and there is no coupling asymmetry for the 4×4 case.

Two $\mathbf{W}_j$ matrices consisting of $\overleftrightarrow{\mathbf{M}}$ eigenvector columns can be written in the following form:

$$\mathbf{W}_1=\tfrac{1}{\delta}\begin{pmatrix}a_{21}\mathbf{I} & -\mathbf{R}\\ -\hat{\mathbf{R}} & a_{11}\mathbf{I}\end{pmatrix},$$
$$\mathbf{W}_2=-\tfrac{1}{\delta}\begin{pmatrix}a_{22}\mathbf{I} & -\mathbf{R}\\ -\hat{\mathbf{R}} & a_{12}\mathbf{I}\end{pmatrix}.$$

The following relation similar to Eq. (33) holds for them:

$$\mathbf{W}_1+\mathbf{W}_2=\mathbf{I}_4.$$

Commutation rules Eq. (51) can be transformed into

$$\begin{matrix}\mathbf{R}(1-u)\mathbf{J}_{21}=u\mathbf{J}_{11}\mathbf{R}\\ \mathbf{R}u\mathbf{J}_{22}=(1-u)\mathbf{J}_{12}\mathbf{R}\end{matrix}. \tag{70}$$

This system has a nontrivial solution only if the following identity holds (see Appendix E):

$$\begin{aligned}&\mathrm{Tr}\,(\mathbf{J}_{21}\mathbf{J}_{22}-\mathbf{J}_{11}\mathbf{J}_{12})=\beta_{11}\gamma_{12}+\beta_{12}\gamma_{11}\\ &-2\alpha_{11}\alpha_{12}-\beta_{22}\gamma_{21}-\beta_{21}\gamma_{22}+2\alpha_{21}\alpha_{22}=0.\end{aligned}$$

Using γ_{ij} definition from Eq. (47), it leads to the following quadratic equation on u:

$$\begin{aligned}&\left(\frac{\beta_{11}}{\beta_{12}}+\frac{\beta_{12}}{\beta_{11}}-\frac{\beta_{22}}{\beta_{21}}-\frac{\beta_{21}}{\beta_{22}}\right)u^2+2\left(\frac{\beta_{21}}{\beta_{22}}-\frac{\beta_{12}}{\beta_{11}}\right)u\\ &+\frac{\beta_{11}}{\beta_{12}}\alpha_{12}^2+\frac{\beta_{12}}{\beta_{11}}\alpha_{11}^2-\frac{\beta_{22}}{\beta_{21}}\alpha_{21}^2-\frac{\beta_{21}}{\beta_{22}}\alpha_{22}^2\\ &+2\alpha_{21}\alpha_{22}-2\alpha_{11}\alpha_{12}=0.\end{aligned} \tag{71}$$

The following correspondence exists between the notations used in the present paper and [3]:

$$\begin{aligned}&\beta_{11}\equiv\beta_{1x},\ \ \beta_{21}\equiv\beta_{1y},\ \ \beta_{12}\equiv\beta_{2x},\ \ \beta_{22}\equiv\beta_{2y},\\ &\alpha_{11}\equiv\alpha_{1x},\ \ \alpha_{21}\equiv\alpha_{1y},\ \ \alpha_{12}\equiv\alpha_{2x},\ \ \alpha_{22}\equiv\alpha_{2y}.\end{aligned}$$

Using it, one can easily prove that Eq. (3.8) in [3] describes the solutions of Eq. (71). Therefore, not only parameters μ_j but also parameter u have the same meaning in both parameterizations.

XII. CONCLUSION

Symmetry properties of 6×6 and 4×4 symplectic matrices have been thoroughly investigated in application to matrix optics in accelerator physics. Twiss parameterization has been developed for the 6×6 case (direct and inverse procedure, along with the emittance concept). The resulting parameterization can be reduced in 4×4 case to the well-known Lebedev-Bogacz parameterization [3]. The intrinsic sign ambiguity of the Twiss parameterization has been studied in detail.

Additional features of the suggested approach are switching from the sixth- to the third-order characteristic equation, from 6×6 to 2×2 matrix multiplication and from complex to real numbers. This allows all the calculations to be performed analytically, as well as to be efficiently implemented in any programming language.

DATA AVAILABILITY

The data that support the findings of this article are openly available [12].

APPENDIX A: RECURRENT MATRIX EIGENVALUE SORTING

Before calculating $\overleftrightarrow{\mathbf{M}}$ eigeivectors, one should find the correspondence between its eigenvalues (found in Sec. IV) and spatial degrees of freedom. One needs a procedure how to define a "measure" of the horizontal, vertical, and longitudinal motion in a pair of $\overleftrightarrow{\mathbf{M}}$ eigenvectors corresponding to the $\hat{\lambda}_j$ eigenvalue. It is obvious that any of their linear combinations is also an $\overleftrightarrow{\mathbf{M}}$ eigenvector corresponding to the same eigenvalue. Vector components 1 and 2 describe the horizontal motion, components 3 and 4 describe the vertical motion and components 5 and 6 correspond to the longitudinal motion. Therefore, for a pair of six-component vectors, we need three real numbers depending on the corresponding vector component pair only, their order on the real axis should be the same for any linear combination of the vectors. The simplest procedure is to form a 6×2 matrix of these vectors and calculate absolute values of the determinants of the resulting three 2×2 blocks in it.

Let us define the *contraction* operation $\{\}$ on an $m\times n$ matrix with even m and n:

$$\{\mathbf{A}\}=\left\{\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1,n-1} & a_{1,n}\\ a_{21} & a_{22} & \cdots & a_{2,n-1} & a_{2,n}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ a_{m-1,1} & a_{m-1,2} & \cdots & a_{m-1,n-1} & a_{m-1,n}\\ a_{m,1} & a_{m,2} & \cdots & a_{m,n-1} & a_{m,n}\end{pmatrix}\right\}$$
$$=\begin{pmatrix} \mathrm{abs}\begin{vmatrix} a_{11} & a_{12}\\ a_{21} & a_{22}\end{vmatrix} & \cdots & \mathrm{abs}\begin{vmatrix} a_{1,n-1} & a_{1,n}\\ a_{2,n-1} & a_{2,n}\end{vmatrix}\\ \vdots & \ddots & \vdots\\ \mathrm{abs}\begin{vmatrix} a_{m-1,1} & a_{m-1,2}\\ a_{m,1} & a_{m,2}\end{vmatrix} & \cdots & \mathrm{abs}\begin{vmatrix} a_{m-1,n-1} & a_{m-1,n}\\ a_{m,n-1} & a_{m,n}\end{vmatrix}\end{pmatrix}, \tag{A1}$$

where abs denotes absolute value. Then, the matrix $\mathbf{V}_1$ in Eq. (25) can be contracted as follows:

$$\{\mathbf{V}_1\}=\tilde{\mathbf{C}}\begin{pmatrix} |c_{11}| & 0 & 0\\ 0 & |c_{22}| & 0\\ 0 & 0 & |c_{33}|\end{pmatrix}, \tag{A2}$$

where

$$\tilde{\mathbf{C}}=\begin{pmatrix} |c_{11}| & |c_{12}| & |c_{13}|\\ |c_{21}| & |c_{22}| & |c_{23}|\\ |c_{31}| & |c_{32}| & |c_{33}|\end{pmatrix}. \tag{A3}$$

The following procedure is recommended for eigenvalue sorting: (i) Obtain $\hat{\lambda}_a$, $\hat{\lambda}_b$, $\hat{\lambda}_c$ eigenvalues according to Eq. (22). (ii) Find c_{ij} from Eq. (30) and form $\tilde{\mathbf{C}}$ matrix according to Eq. (A3) in $\{a,b,c\}$ indices. (iii) Sort $\tilde{\mathbf{C}}$ columns to maximize its trace. If more than one solution is possible, then any of them may be chosen. (iv) Performed permutations define the correspondence between the $\{a,b,c\}$ and $\{1,2,3\}$ indices.

APPENDIX B: DEGENERATED CASE

The approach proposed in the present paper is, in general, not applicable to the case when one of the recurrent matrix eigenvalues is degenerated more than twice. To show this fact, it is enough to consider a simple example in the 4×4 case. The sample lattice is a FODO cell with symmetric drifts of the length L and thin quadrupole lenses of the integrated strengths P and $-P$, tilted by angle φ around the longitudinal axis.

The approach proposed here is to switch to the recurrent matrix $\overleftrightarrow{\mathbf{M}}$ and then calculate the coupling matrix and W matrices from it. However, in the example given above $\overleftrightarrow{\mathbf{M}}=(2-L^2P^2)\mathbf{I}_4$ and all information about the coupling matrix elements has been lost at this point. Instead of switching to $\overleftrightarrow{\mathbf{M}}$ one should introduce an infinitezimal difference between the absolute values of the quadrupole strengths and calculate the coupling matrix elements using a limit transition:

$$\mathbf{U}=\begin{pmatrix} \cos^2\varphi & \sin^2\varphi\\ \sin^2\varphi & \cos^2\varphi\end{pmatrix}.$$

A universal approach to degenerated cases in terms of the proposed theory is still to be found.

APPENDIX C: ADDITIONAL W-MATRIX PROPERTIES

All $\mathbf{W}_{ij}$ can be expressed through only three of them. Combining Eqs. (31) and (34), one can express all W matrices through $\mathbf{W}_{ii}$, $\mathbf{W}_{i\vec{i}}$, or $\mathbf{W}_{i\overleftarrow{i}}$. The calculations are similar for all these options. However, for $\mathbf{W}_{ii}$, the resulting expressions are more compact, therefore intermediate calculations will be shown only for that option. So, the following equations on $\mathbf{W}_{i\vec{i}}$ and $\mathbf{W}_{i\overleftarrow{i}}$ can be obtained:

$$\begin{aligned} &u_{\vec{i}\vec{i}}u_{\bar{i}\vec{i}}u_{\bar{i}\bar{i}}\mathbf{W}_{\vec{i}\vec{i}} + (\hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}})\hat{\mathbf{W}}_{\vec{i}\vec{i}}\mathbf{W}_{ii} \\ &\quad = u_{\vec{i}\vec{i}}u_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}} - u_{\bar{i}\bar{i}}u_{\vec{i}\vec{i}}(u_{\vec{i}\bar{i}} + u_{\bar{i}\vec{i}})\mathbf{W}_{ii}, \\ &u_{\vec{i}\vec{i}}u_{\bar{i}\vec{i}}u_{\bar{i}\bar{i}}\mathbf{W}_{\vec{i}\bar{i}} + \mathbf{W}_{ii}\hat{\mathbf{W}}_{\vec{i}\bar{i}}(\hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}}) \\ &\quad = u_{\vec{i}\vec{i}}u_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}} - u_{\bar{i}\bar{i}}u_{\vec{i}\vec{i}}(u_{\vec{i}\bar{i}} + u_{\bar{i}\vec{i}})\mathbf{W}_{ii}. \end{aligned} \tag{C1}$$

Each of them is a system of four linear equations. These systems can be solved directly, however, a much simpler way exists. One may note from Eq. (C1) that all $\mathbf{W}_{\vec{i}\vec{i}}$ and $\mathbf{W}_{\vec{i}\bar{i}}$ can be found as linear combinations of $\mathbf{W}_{ii}$ and $\hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}}$. Finally, for each of the three options, one obtains

$$\begin{aligned} l\,\mathbf{W}_{\vec{i}\vec{i}} &= \hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}} - u_{\bar{i}\bar{i}}\mathbf{W}_{ii} \\ l\,\mathbf{W}_{\vec{i}\bar{i}} &= -\hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}} + u_{\bar{i}\bar{i}}\mathbf{W}_{ii} \end{aligned}, \tag{C2a}$$

$$\begin{aligned} l_+\mathbf{W}_{ii} &= \hat{\mathbf{W}}_{\bar{i}\vec{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}} - u_{\bar{i}\vec{i}}\mathbf{W}_{\vec{i}\bar{i}} \\ l_+\mathbf{W}_{\vec{i}\bar{i}} &= -\hat{\mathbf{W}}_{\bar{i}\vec{i}}\hat{\mathbf{W}}_{\bar{i}\bar{i}} + u_{\bar{i}\bar{i}}\mathbf{W}_{\vec{i}\bar{i}} \end{aligned}, \tag{C2b}$$

$$\begin{aligned} l_-\mathbf{W}_{ii} &= \hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\vec{i}\bar{i}} - u_{\bar{i}\vec{i}}\mathbf{W}_{\vec{i}\vec{i}} \\ l_-\mathbf{W}_{\vec{i}\vec{i}} &= -\hat{\mathbf{W}}_{\bar{i}\bar{i}}\hat{\mathbf{W}}_{\vec{i}\bar{i}} + u_{\bar{i}\bar{i}}\mathbf{W}_{\vec{i}\vec{i}} \end{aligned}, \tag{C2c}$$

where

$$l_\pm = \frac{1}{2}(1 \pm l - u_{11} - u_{22} - u_{33}).$$

APPENDIX D: COMMUTATION MATRIX EQUATIONS

The following matrix equation appears several times throughout the study:

$$\mathbf{XA} = \mathbf{BX}, \quad \text{where } |\mathbf{A}| = |\mathbf{B}| = d, \tag{D1}$$

d is a constant, $\mathbf{A}$ and $\mathbf{B}$ are constant 2×2 matrices, and $\mathbf{X}$ is a 2×2 matrix to be found. In the present paper, they are referred to as *commutation* 2×2 *matrix equations*. Such an equation can be regarded as a system of four homogeneous linear equations with the following matrix:

$$\mathbf{\Delta} = \begin{pmatrix} a_{11}-b_{11} & a_{21} & -b_{12} & 0 \\ a_{12} & a_{22}-b_{11} & 0 & -b_{12} \\ -b_{21} & 0 & a_{11}-b_{22} & a_{21} \\ 0 & -b_{21} & a_{12} & a_{22}-b_{22} \end{pmatrix}, \tag{D2}$$

where a_{ij} and b_{ij} are corresponding elements of $\mathbf{A}$ and $\mathbf{B}$ matrices. Its determinant can be expressed in a compact form:

$$|\mathbf{\Delta}| = d\,(\mathrm{Tr}\,\mathbf{A} - \mathrm{Tr}\,\mathbf{B})^2.$$

This system has a nontrivial solution if and only if $|\mathbf{\Delta}| = 0$. The case $d = 0$ will not be studied separately because $|\mathbf{\Delta}|$ can be made identically equal to zero by switching from matrices $\mathbf{A}$ and $\mathbf{B}$ to their traceless parts.[6] Then, Eq. (D1) transforms into

$$\mathbf{XA} = \mathbf{BX}, \quad \text{where } |\mathbf{A}| = |\mathbf{B}| = d,\ \mathrm{Tr}\,\mathbf{A} = \mathrm{Tr}\,\mathbf{B} = 0. \tag{D3}$$

This corresponds to the substitutions $a_{22} = -a_{11}$ and $b_{22} = -b_{11}$ in Eq. (D2). After that, one can easily check that $\mathrm{rank}\,\mathbf{\Delta} = 0$ if and only if $\mathbf{A} = \mathbf{B} = \mathbf{0}$, otherwise $\mathrm{rank}\,\mathbf{\Delta} = 2$. It is always possible for any $\mathbf{A}$ and $\mathbf{B}$ to choose two constant matrices $\mathbf{\Phi}$ and $\mathbf{\Psi}$ from the given set

$$\mathbf{\Phi}, \mathbf{\Psi} \in \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right\}, \quad \mathbf{\Phi} \neq \mathbf{\Psi} \tag{D4}$$

to express $\mathbf{X}$ in the following form:

$$\mathbf{X} = \begin{cases} \text{arbitrary}, & \mathbf{A} = \mathbf{B} = \mathbf{0} \\ \xi(\mathbf{\Phi A} + \mathbf{B\Phi}) + \eta(\mathbf{\Psi A} + \mathbf{B\Psi}), & \text{otherwise} \end{cases} \tag{D5}$$

Although in simulations the same results with sufficient precision have been always obtained for arbitrary choice of $\mathbf{\Phi}$ and $\mathbf{\Psi}$, the following optimization procedure can be proposed. Two matrices are linearly dependent if and only if each element pair in one of them, regarded as a 2D vector, is collinear to the corresponding pair in the second one. Therefore, a *linear independency measure* $\Delta_\parallel(\mathbf{A}, \mathbf{B})$ can be introduced for 2×2 matrices $\mathbf{A}$ and $\mathbf{B}$:

$$\begin{aligned} \Delta_\parallel(\mathbf{A}, \mathbf{B}) = {} & (a_{11}b_{12} - a_{12}b_{11})^2 + (a_{21}b_{22} - a_{22}b_{21})^2 + \\ & (a_{11}b_{21} - a_{21}b_{11})^2 + (a_{12}b_{22} - a_{22}b_{12})^2 + \\ & (a_{11}b_{22} - a_{22}b_{11})^2 + (a_{12}b_{21} - a_{21}b_{12})^2, \end{aligned}$$

[6] For a 2×2 matrix $\mathbf{A}$, extraction of the traceless part means the following:

$$\mathbf{A} \mapsto \mathbf{A} - \frac{\mathrm{Tr}\,\mathbf{A}}{2}\mathbf{I}.$$

Here we do not introduce a special notation for this operation to avoid additional complication of the formulas.
If $\mathbf{A}$ and $\mathbf{B}$ are 2×2 traceless matrices, then

1. $\hat{\mathbf{A}} = -\mathbf{A}$,
2. $\mathbf{A}^2 = -|\mathbf{A}|\mathbf{I}$,
3. $\mathbf{AB} + \mathbf{BA} = \mathrm{Tr}\,(\mathbf{AB})\mathbf{I}$.

These properties are widely used throughout the Appendices part of the present paper.

where a_{ij} and b_{ij} are $\mathbf{A}$ and $\mathbf{B}$ elements. So, $\mathbf{\Phi}$ and $\mathbf{\Psi}$ in Eq. (D4) should be chosen to maximize $\Delta_{\|}(\mathbf{\Phi A}+\mathbf{B\Phi}, \mathbf{\Psi A}+\mathbf{B\Psi})$.

APPENDIX E: SYSTEM OF THREE COMMUTATION MATRIX EQUATIONS

A system of commutation 2×2 matrix equations for three different matrices $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$ with zero sum and known determinants should be studied separately:

$$\begin{gathered}\mathbf{XA}=\mathbf{BX}, |\mathbf{X}|=x\\ \mathbf{YC}=\mathbf{DY}, |\mathbf{Y}|=y\\ \mathbf{ZE}=\mathbf{FZ}, |\mathbf{Z}|=z\\ \mathbf{X}+\mathbf{Y}+\mathbf{Z}=\mathbf{0}\end{gathered}, \tag{E1}$$

where

$$|\mathbf{A}|=|\mathbf{B}|=x^2,\ |\mathbf{C}|=|\mathbf{D}|=y^2,\ |\mathbf{E}|=|\mathbf{F}|=z^2,$$
$$\mathrm{Tr}\,\mathbf{A}=\mathrm{Tr}\,\mathbf{B}=\mathrm{Tr}\,\mathbf{C}=\mathrm{Tr}\,\mathbf{D}=\mathrm{Tr}\,\mathbf{E}=\mathrm{Tr}\,\mathbf{F}=0,$$

x, y, z are constants, $\mathbf{A},\ldots,\mathbf{F}$ are constant 2×2 matrices. Multiplying the first two equations by $\mathbf{B}$, $\mathbf{D}$ on the left and by $\mathbf{A}$, $\mathbf{C}$ on the right and summing up the results, one can easily express $\mathbf{X}$ and $\mathbf{Y}$ through $\mathbf{Z}$:

$$\begin{gathered}\tau\mathbf{X}=(\mathbf{DZ}-\mathbf{ZC})\mathbf{A}+\mathbf{B}(\mathbf{DZ}-\mathbf{ZC})\\ \tau\mathbf{Y}=(\mathbf{BZ}-\mathbf{ZA})\mathbf{C}+\mathbf{D}(\mathbf{BZ}-\mathbf{ZA})\end{gathered}, \tag{E2}$$

where

$$\tau=\mathrm{Tr}\,(\mathbf{AC}-\mathbf{BD}).$$

For better precision, before solving Eq. (E1), one should find and apply the same permutation to the $\{\mathbf{A},\mathbf{C},\mathbf{E}\}$, $\{\mathbf{B},\mathbf{D},\mathbf{F}\}$, and $\{x,y,z\}$ lists, which maximizes $|\tau|$. Then the inverse permutation should be applied in the end to the resulting $\{\mathbf{X},\mathbf{Y},\mathbf{Z}\}$ list.

Subtracting determinants of both parts of Eq. (E2) and combining the result with the third equation of Eq. (E1), one obtains an equation system on $\mathbf{Z}$:

$$\begin{gathered}\mathbf{ZE}=\mathbf{FZ}\\ |\mathbf{Z}|=z\\ \tau\mathrm{Tr}\,(\mathbf{ZC}\hat{\mathbf{Z}}\mathbf{B}-\mathbf{ZA}\hat{\mathbf{Z}}\mathbf{D})=\tau^2(x-y)\end{gathered}. \tag{E3}$$

It is important for the present study to distinguish between the two cases: when this system has either infinite or finite set of solutions. If $\mathbf{E}=\mathbf{F}=\mathbf{0}$, then the set is infinite because the first equation does not impose any restrictions on $\mathbf{Z}$ elements. In all other cases, solution of the first equation is given in Eq. (D5):

$$\mathbf{Z}=\xi\mathbf{G}+\eta\mathbf{H},$$

where

$$\mathbf{G}=\mathbf{\Phi E}+\mathbf{F\Phi},\qquad \mathbf{H}=\mathbf{\Psi E}+\mathbf{F\Psi},$$

ξ and η are free parameters, $\mathbf{\Phi}$ and $\mathbf{\Psi}$ are chosen from Eq. (D4) to minimize $\Delta_{\|}(\mathbf{G},\mathbf{H})$. Then the rest of Eq. (E3) forms a system of two quadratic equations on these two parameters:

$$\begin{gathered}a_1\xi^2+2b_1\xi\eta+c_1\eta^2=r_1\\ a_2\xi^2+2b_2\xi\eta+c_2\eta^2=r_2\end{gathered}, \tag{E4}$$

where

$$\begin{aligned}a_1&=-\mathrm{Tr}\,(\mathbf{E}\hat{\mathbf{\Phi}}\mathbf{F\Phi}),\\ b_1&=\mathrm{Tr}\,(z^2\mathbf{\Phi}\hat{\mathbf{\Psi}}-\mathbf{E}\hat{\mathbf{\Psi}}\mathbf{F\Phi}),\\ c_1&=-\mathrm{Tr}\,(\mathbf{E}\hat{\mathbf{\Psi}}\mathbf{F\Psi}),\\ r_1&=z,\\ a_2&=\tau\mathrm{Tr}\,(\mathbf{GC}\hat{\mathbf{G}}\mathbf{B}-\mathbf{GA}\hat{\mathbf{G}}\mathbf{D}),\\ b_2&=\tau\mathrm{Tr}\,(\mathbf{GC}\hat{\mathbf{H}}\mathbf{B}-\mathbf{GA}\hat{\mathbf{H}}\mathbf{D}),\\ c_2&=\tau\mathrm{Tr}\,(\mathbf{HC}\hat{\mathbf{H}}\mathbf{B}-\mathbf{HA}\hat{\mathbf{H}}\mathbf{D}),\\ r_2&=\tau^2(x-y).\end{aligned}$$

If $r_1=r_2=0$, then there are either no solutions (this case cannot be realized in the present study), single solution $(\xi;\eta)=(0;0)$, or infinite number of solutions. Otherwise the system Eq. (E4) has a finite number of solutions if and only if at least one coefficient in the combined equation is nonzero:

$$a_3\xi^2+2b_3\xi\eta+c_3\eta^2=0, \tag{E5}$$

where

$$a_3=a_1r_2-a_2r_1,\qquad b_3=b_1r_2-b_2r_1,$$
$$c_3=c_1r_2-c_2r_1.$$

Finally, either ξ/η or η/ξ can be found from Eq. (E5) and substituted into Eq. (E4).

APPENDIX F: SYSTEM OF TWO COMMUTATION MATRIX EQUATIONS

If one of the matrices of interest in Eq. (E1) is put to be zero, then this system can be reduced to the following form:

$$\begin{gathered}\mathbf{XA}=\mathbf{BX}\\ \mathbf{XC}=\mathbf{DX}\\ |\mathbf{X}|=x\end{gathered}\qquad \begin{gathered}\text{where}\\ |\mathbf{A}|=|\mathbf{B}|=|\mathbf{C}|=|\mathbf{D}|=x^2,\\ \mathrm{Tr}\,\mathbf{A}=\mathrm{Tr}\,\mathbf{B}=\mathrm{Tr}\,\mathbf{C}=\mathrm{Tr}\,\mathbf{D}=0,\end{gathered} \tag{F1}$$

$\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$ are constant 2×2 matrices and $\mathbf{X}$ is a 2×2 matrix to be found. Using the same approach as in deriving Eq. (E2), one immediately obtains $\tau\mathbf{X}=\mathbf{0}$. This means that Eq. (F1) has a nontrivial solution if and only if $\tau=0$. Using

this condition, the solution of Eq. (F1) can be expressed in the following form:

$$\mathbf{X} = \begin{cases} k[(\mathbf{D}-\mathbf{C})\mathbf{A}+\mathbf{B}(\mathbf{D}-\mathbf{C})] = \\ k[(\mathbf{A}-\mathbf{B})\mathbf{C}+\mathbf{D}(\mathbf{A}-\mathbf{B})] \\ \mathbf{0}, \end{cases} \quad \begin{array}{l} \mathrm{Tr}\,(\mathbf{AC}-\mathbf{BD}) = 0, \\ \\ \text{otherwise}, \end{array} \tag{F2}$$

where

$$k = \pm\sqrt{\frac{|x|}{|(\mathbf{D}-\mathbf{C})\mathbf{A}+\mathbf{B}(\mathbf{D}-\mathbf{C})|}}.$$

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