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Analytical methods for describing charged particle dynamics in general focusing lattices using generalized Courant-Snyder theory

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Abstract

The dynamics of charged particles in general linear focusing lattices with quadrupole, skew-quadrupole, dipole, and solenoidal components, as well as torsion of the fiducial orbit and variation of beam energy is parameterized using a generalized Courant-Snyder (CS) theory, which extends the original CS theory for one degree of freedom to higher dimensions. The envelope function is generalized into an envelope matrix, and the phase advance is generalized into a 4D symplectic rotation, or an $U(2)$ element. The 1D envelope equation, also known as the Ermakov-Milne-Pinney equation in quantum mechanics, is generalized to an envelope matrix equation in higher dimensions. Other components of the original CS theory, such as the transfer matrix, Twiss functions, and CS invariant (also known as the Lewis invariant) all have their counterparts, with remarkably similar expressions, in the generalized theory. The gauge group structure of the generalized theory is analyzed. By fixing the gauge freedom with a desired symmetry, the generalized CS parameterization assumes the form of the modified Iwasawa decomposition, whose importance in phase space optics and phase space quantum mechanics has been recently realized. This gauge fixing also symmetrizes the generalized envelope equation and express the theory using only the generalized Twiss function β. The generalized phase advance completely determines the spectral and structural stability properties of a general focusing lattice. For structural stability, the generalized CS theory enables application of the Krein-Moser theory to greatly simplify the stability analysis. The generalized CS theory provides an effective tool to study coupled dynamics and to discover more optimized lattice design in the larger parameter space of general focusing lattices.

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I. INTRODUCTION

In accelerators and storage rings, charged particles are confined transversely by electromagnetic focusing lattices. Many different kinds of focusing lattice have been successfully designed and implemented. The fundamental theoretical tool in designing an uncoupled quadrupole lattice is the Courant-Snyder (CS) theory [1], which can be summarized as follows. For a given set of focusing lattice in the $x-$ and $y-$directions $\kappa_x(t)$ and $\kappa_y(t)$, particle's dynamics is governed by the oscillation equation

$$\ddot{q} + \kappa_q(t) q = 0 \,, \tag{1}$$

where q represents one of the transverse coordinates, either x or y. Solution of Eq. (1) can be expressed as a symplectic linear map $M(t)$ that advances the phase space coordinates

$$\begin{pmatrix} q \\ \dot{q} \end{pmatrix} = M\left(t\right) \begin{pmatrix} q_0 \\ \dot{q}_0 \end{pmatrix} . \tag{2}$$

In CS theory, the linear map $M(t)$ is given as

$$M\left(t\right) = \begin{pmatrix} \sqrt{\dfrac{\beta}{\beta_0}}\left[\cos\phi + \alpha_0 \sin\phi\right] & \sqrt{\beta\beta_0}\sin\phi \\ -\dfrac{1+\alpha\alpha_0}{\sqrt{\beta\beta_0}}\sin\phi + \dfrac{\alpha_0 - \alpha}{\sqrt{\beta\beta_0}}\cos\phi & \sqrt{\dfrac{\beta_0}{\beta}}\left[\cos\phi - \alpha\sin\phi\right] \end{pmatrix} , \tag{3}$$

where $\alpha\left(t\right)$ and $\beta\left(t\right)$ are two of the so-called Twiss parameters, and $\phi\left(t\right)$ is the phase advance. They are defined by an envelope function $w\left(t\right)$ as

$$\beta\left(t\right) = w^2\left(t\right) \,, \tag{4}$$

$$\alpha\left(t\right) = -w\dot{w} \,, \tag{5}$$

$$\phi\left(t\right) = \int_0^t \frac{dt}{\beta\left(t\right)} \,, \tag{6}$$

and the envelope function $w\left(t\right)$ is determined by the envelope equation

$$\ddot{w} + \kappa_q\left(t\right) w = w^{-3} \,. \tag{7}$$

In Eq. (3), $q_0 = q\left(t=0\right)$, $\dot{q}_0 = \dot{q}\left(t=0\right)$, $\beta_0 = \beta\left(t=0\right)$, and $\alpha_0 = \alpha\left(t=0\right)$ are the initial conditions at $t = 0$.

Associated with the dynamics of Eq. (1), there exists a constant of motion, I_{CS}, known as the Courant-Synder invariant

$$I_{CS} = \frac{q^2}{w^2} + (w\dot{q} - \dot{w}q)^2 = (q, \dot{q}) \begin{pmatrix} \gamma & \alpha \\ \alpha & \beta \end{pmatrix} \begin{pmatrix} q \\ \dot{q} \end{pmatrix} , \tag{8}$$

$$\gamma(t) \equiv w^{-2} + \dot{w}^2 . \tag{9}$$

Here $\gamma(t)$ is the third Twiss parameter. It turns out that the transfer matrix $M(t)$ can be decomposed into the elegant form [2]

$$M(t) = \begin{pmatrix} w & 0 \\ \dot{w} & \dfrac{1}{w} \end{pmatrix} \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} w_0^{-1} & 0 \\ -\dot{w}_0 & w_0 \end{pmatrix} , \tag{10}$$

which seems to indicate a certain structure for $M(t)$.

The CS theory can be viewed as a parameterization method of the time-dependent 2×2 symplectic matrix $M(t)$ for a standard uncoupled lattice. Not surprisingly, there exist other parameterization schemes mathematically. Why is the CS parameterization preferable? This is because it describes the physics of charged particle dynamics. The main components of the CS theory, i.e., the phase advance, the envelope equation, the transfer matrix, and the CS invariant are physical quantities describing the dynamics of the particles. For example, the CS invariant defines the emittance in phase space, and the envelope function describes the transverse dimensions in configuration space. This theoretical framework also makes it possible to investigate collective effects associated with high-intensity beams, such as in the construction of the Kapchinskij-Vladimirskij distribution [3–5].

However, the CS theory can only be applied to the $x-$ or $y-$dynamics separately for the ideal case of uncoupled quadrupole focusing lattices. In realistic accelerators, there exist bending magnets, torsion of the design orbit (fiducial orbit), and skew-quadrupole components, which are introduced intentionally or by misalignment [6, 7]. Solenoidal magnets are also used in certain applications [8]. When these additional components are included, the transverse dynamics in the $x-$ and $y-$directions are coupled, and the focusing force depends on the transverse momentum as well. In this most general case, the transfer matrix $M(t)$ is a time-dependent 4×4 symplectic matrix, which has 10 time-dependent parameters and admits many different schemes for parameterization. The first set of parameterization schemes for $M(t)$ were developed by Teng and Edwards [9–11] and Ripken [12–14], some of

which have been adopted in lattice design and particle tracking codes, such as the MAD code [15, 16]. A class of different parameterizations by directly generalizing the Twiss parameters to higher dimensions has also been developed by Dattoli, et al. [17–19]. However, in contrast to the original CS theory, these parameterization schemes are designed from mathematical considerations, and fail to connect with physical parameters of the beam. The elegant and much-needed connection with the physics of beam dynamics in the original CS theory for one degree of freedom is not transparent in these parameterization schemes. This is probably why there is no *de facto* standard yet adopted by the accelerator community. Another main reason is that for most present-day accelerators and rings, the transverse dynamics are so nearly decoupled that perturbative treatment often works satisfactorily. Even for lattices with strong coupling, elementary methods can be used to analyze the dynamics, even though the calculation often become rather involved and requires diligence and patience.

In a recent Letter [20], we reported the development of a generalized CS theory for focusing lattices with the most general form in Eq. (11), including bending magnets, torsion of the design orbit, and solenoidal magnets, in addition to quadrupole and skew-quadrupole components. In this generalized theory, the physics elements of the original CS theory, i.e., the phase advance, the envelope equation, the transfer matrix, and the CS invariant are all generalized to the 2D coupled case with identical structure. This new development also generalizes our previous results for coupled dynamics including only a skew-quadrupole lattice component [21–24]. In this paper, we give a detailed derivation of the generalized CS theory reported in Ref. [20], describe the theoretical structure of the theory in terms of gauge freedoms and group decomposition, and demonstrate the application of the theory in stability analysis.

II. THEORETICAL MODEL AND SUMMARY OF RESULTS

In this section, we outline the theoretical methods used and summarize the main results obtained in this paper. As discussed in Sec. I, when realistic components such as skew-quadrupoles, bending magnets, torsion of the design orbit, solenoidal magnets are included, in addition to the standard quadrupole components, the transverse dynamics in the $x-$ and $y-$directions are coupled, and the focusing force depends on the transverse momentum. In this case, the linear dynamics of a charged particle relative to the fiducial orbit are governed

by a general time-dependent Hamiltonian [25] of the form

$$H = \frac{1}{2} z^T A z \,, \quad A = \begin{pmatrix} \kappa\,(t) & R\,(t) \\ R\,(t)^T & m^{-1}\,(t) \end{pmatrix} . \tag{11}$$

Here, $z = (x, y, p_x, p_y)^T$ are the transverse phase space coordinates, and $\kappa(t)$, $R\,(t)$ and $m^{-1}\,(t)$ are time-dependent 2×2 matrices. The matrices A, $\kappa(t)$ and $m^{-1}\,(t)$ are also symmetric. In this most general Hamiltonian, the skew-quadrupole and dipole components are included in the off-diagonal terms of the $\kappa\,(t)$ matrix, and the solenoidal component and the torsion of the fiducial orbit are included in the $R\,(t)$ matrix. There are several different methods to include the effect of torsion, which were reviewed by Hoffstaetter [26]. Typically, Frenet-Serret coordinates along the fiducial orbit is used. When the fiducial orbit is straight, the Frenet-Serret coordinates are not uniquely defined. In this case, we can choose any particular set of Frenet-Serret coordinates in the straight section, as long it is smoothly connected to those in the curved sections. The variation of beam energy along the fiducial orbit is reflected in the mass matrix $m^{-1}\,(t)$, which is allowed to be any real symmetric matrix for complete generality. The transfer matrix $M(t)$ corresponding to H is a time-dependent 4×4 symplectic matrix, which has 10 time-dependent parameters. Our goal is to develop a generalized Courant-Snyder parameterization method for $M(t)$, which has the same elegant structure and direct connection to beam dynamics as the original Courant-Snyder theory for one degree of freedom.

We will use a time-dependent symplectic transformation technique [21, 24, 27] to analyze the charged particle dynamics governed by the Hamiltonian given in Eq. (11). This technique is described in Sec. III. The concept of scalar envelope function is generalized to a 2×2 envelope matrix, and the envelope equation in 2×2 matrix form is developed [see Eq. (36)]. In the original CS theory, the envelope equation (7) is one dimensional and plays a central role. It also has been discovered or re-discovered many times [28–32] in other branches of physics. In quantum physics, it is known as the Ermakov-Milne-Pinney equation [28–30], which has been utilized to study 1D time-dependent quantum systems [33, 34] and associated non-adiabatic Berry phases [35]. A brief account of the history of the 1D envelope equation can be found in Ref. [36]. We expect the generalization of the envelope equation to higher dimensions for the most general Hamiltonian to have applications in areas other than beam physics as well. The 1D CS invariant given by Eq. (8), also known as the Lewis invariant

[31, 32] in quantum physics, is generalized to higher dimensions in Eqs. (44) and (45).

Also in Sec. IV, the 1D phase advance is generalized to a time-dependent matrix P, which belongs to the symplectic rotation group $Sp(4) \bigcap SO(4) = U(2)$. Here, $Sp(4)$, $SO(4)$, and $U(2)$ denote the groups of 4×4 symplectic matrices, 4×4 rotation matrices, and 2×2 unitary matrices, respectively. For dynamics with one degree of freedom, the phase advance is naturally an angle (an element of $SO(2)$) in the 2D phase space. For dynamics with two degrees of freedom, the phase space is 4D, and it is tempting to represent the phase advance by two angles. This is what has been adopted in previous parameterization schemes. From the viewpoint of theoretical physics and geometry, however, it is more natural to represent the phase advance for dynamics with two degrees of freedom by a 4D rotation (an element of $SO(4)$), which is not equivalent to two 2D rotations. Because of the symplectic nature of the Hamiltonian dynamics, the generalized phase advance in higher dimensions thus belongs to the symplectic rotation group. Of course, one can adopt different views on this. In the normal form analysis of accelerator rings, the 4D transfer matrix is reduced to a 2D rotation after block diagonalization. In a sense, we can compare coupled betatron motion to the Dirac equation. In a fully quantum mechanical limit, the only correct approach is to treat electrons and positrons as inextricably coupled; only the 4D approach is permissible in this limit. But in the accelerator physics, we routinely treat electrons and positrons as completely separate entities, and two 2D descriptions are adopted without much hesitation.

The generalized decomposition for the symplectic map $M(t)$ is given by Eq. (43), which has exactly the same structure as the original 1D CS theory given by Eq. (10). In addition to its aesthetic elegance, the generalized CS theory provides an effective tool to describe the beam dynamics governed by the most general Hamiltonian. The 2×2 envelope matrix w defines the transverse dimension of the beam, and the generalized CS invariant defines the emittance. These components of the generalized CS theory are derived in detail in Sec. IV. For the present application to beam transverse dynamics, there are two degrees of freedom. But the theory developed is valid for any degree of freedom. For a system with n-degrees of freedom, the time-dependent matrix $A(t)$ specifying the Hamiltonian in Eq. (11) will be $2n \times 2n$, the envelope matrix will be $n \times n$, and the phase advance will belong to $Sp(2n) \bigcap SO(2n) = U(n)$.

In Sec. V, we investigate the group structure of the generalized CS theory, which is built on the decomposition of the time-dependent symplectic coordinate transformation G

in the form of Eq. (42). There exists a gauge freedom in this decomposition specified by a 2D rotation element $c \in SO(2)$ for every t. The transfer map $M(t)$ is independent of this gauge. By fixing the gauge freedom with a desired symmetry, the decomposition of G as PS assumes the form of the modified Iwasawa decomposition (or pre-Iwasawa decomposition), whose importance in phase space optics [37, 38] and phase space quantum mechanics [39] has been recently realized. This specific gauge fixing also symmetrizes the generalized envelope equation and express the theory using only the generalized Twiss function β. For a symplectic matrix, the modified Iwasawa decomposition is equivalent to the well-known Iwasawa decomposition for a semi-simple Lie group [40]. However, the unique feature of the theory described here is that the decomposition is constructed as a function of time, and from the viewpoint of dynamics using the generalized envelope equation. Nevertheless, it is a pleasant surprise to find the deep connection between the original CS theory for charged particle dynamics [1] and the Iwasawa decomposition for Lie groups [40], two theoretical formalisms developed concurrently. This connection also demonstrates that beam dynamics, phase space optics and quantum dynamics have a similar theoretical structure at the fundamental level. In order to satisfy the symmetry requirement of the modified Iwasawa decomposition, the gauge freedom need to be selected locally as a function of time, which is the characteristics of gauge theories in theoretical physics. This procedure also results in a symmetrized envelope equation in terms of the generalized Twiss parameter β, which is a symmetric, positive-definite matrix. The beam dimensions and emittance can be expressed using the β matrix only.

We show in Sec. VI how the generalized CS theory can be used to analyze the stability of a charge particle dynamics in realistic accelerators with quadrupole, skew-quadrupole, dipole, and solenoidal components, as well as torsion of the fiducial orbit and variation of beam energy. It turns out that the generalized phase advance as a symplectic rotation completely determines the spectral and structural stability properties of the general lattice after a matched solution of the envelope equation is found. For structural stability, the generalized CS theory enables us to apply the Krein-Moser theory [41–45] to greatly simplify the stability analysis. This general result includes the well-known stability criterion for sum/difference resonances for uncoupled quadrupole lattices as a special case.

III. METHOD OF TIME-DEPENDENT CANONICAL TRANSFORMATION

We will construct the generalized Courant-Snyder theory for the general focusing lattice given by Eq. (11) using a method of time-dependent canonical coordinate transformation. Let's consider a linear, time-dependent Hamiltonian system with n-degrees of freedom

$$H = \frac{1}{2} z^T A(t) z \,, \tag{12}$$
$$z = (x_1, x_2, ..., x_n, p_1, p_2, ..., p_n)^T \,.$$

Here, $A(t)$ is a $2n \times 2n$ time-dependent, symmetric matrix. The Hamiltonian in Eq. ((11)) has this form with $n = 2$. The basic idea is to introduce a time-dependent linear canonical transformation [27]

$$\bar{z} = S(t) z \,, \tag{13}$$

such that in the new coordinates $\bar{z}$, the transformed Hamiltonian has the desired form

$$\bar{H} = \frac{1}{2} \bar{z}^T \bar{A}(t) \bar{z} \,, \tag{14}$$

where $\bar{A}(t)$ is a targeted symmetric matrix. Because the transformation (13) is canonical, it requires that

$$SJS^T = J \,, \tag{15}$$

Here, J the $2n \times 2n$ unit symplectic matrix of order $2n$,

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \,, \tag{16}$$

and I is the $n \times n$ unit matrix. Equation (15) implies that S is a symplectic matrix. In addition, it needs to satisfy a differential equation, which can be derived as follows. Hamilton's equation for z is given by

$$\dot{z} = J \nabla H \,, \tag{17}$$

Using index notation, Eq. (17) becomes

$$\dot{z}_j = J_{ij} \frac{\partial H}{\partial z_j} = \frac{1}{2} J_{ij} \left(\delta_{lj} A_{lm} z_m + z_l A_{lk} \delta_{kj} \right)$$
$$= \frac{1}{2} J_{ij} \left(A_{jm} + A_{mj} \right) z_m = J A_{jm} z_m \,. \tag{18}$$

Switching back to matrix notation, Eq. (18) can be expressed as

$$\dot{z} = JAz\,. \tag{19}$$

Similarly,

$$\dot{\bar{z}} = J\bar{A}\bar{z} = J\bar{A}Sz\,. \tag{20}$$

Meanwhile, $\dot{\bar{z}}$ can be directly calculated from Eq. (13) by taking a time-derivative, which gives

$$\dot{\bar{z}} = \dot{S}z + S\dot{z} = \left(\dot{S} + SJA\right)z\,. \tag{21}$$

Combining Eqs. (20) and (21) gives the differential equation for S

$$\dot{S} = \left(J\bar{A}S - SJA\right)\,. \tag{22}$$

The remarkable feature of the canonical transformation S is that it is always symplectic, if S is initially symplectic at $t = 0$. This assertion can be proved by two methods. For the first proof, we follow Leach [27] and consider the dynamics of the matrix $K = SJS^T$,

$$\begin{aligned}\dot{K} &= \dot{S}JS^T + SJ\dot{S}^T \\ &= \left[\left(J\bar{A}S - SJA\right)JS^T + SJ\left(-S\bar{A}J + AJS^T\right)\right] \\ &= \left[J\bar{A}SJS^T - SJS^T\bar{A}J\right] = \left[J\bar{A}K - K\bar{A}J\right]\,.\end{aligned} \tag{23}$$

Equation (23) has a fixed point at $K = J$. If $S(t = 0)$ is symplectic, *i.e.*, $K\,(t = 0) = J$, then $\dot{K} = 0$ and $K = J$ for all t, and S is symplectic for all t. A more geometric proof can be given from the viewpoint of the flow of S. Because A is symmetric, we have $JJ\bar{A} - \bar{A}^T JJ = 0$, which indicates that $J\bar{A}$ belongs to the Lie algebra $sp\,(2n, R)$. We now show that if S is symplectic at a given t, then $J\bar{A}S$ belongs to the tangent space of $Sp\,(2n, R)$ at S, i.e., $J\bar{A}S \in T_S SP\,(2n, R)$. Let's examine the Lie group right action: $S : a \mapsto aS$ for any a in $Sp\,(2n, R)$, and the associated tangent map

$$T_S :\ T_a Sp\,(2n, R) \to T_{aS} Sp\,(2n, R)\,. \tag{24}$$

It is evident that $J\bar{A}S$ is the image of the Lie algebra element $J\bar{A}$ under the tangential map T_S. This means that $J\bar{A}S$ is a vector tangential to the space of $Sp\,(2n, R)$ at S, if S is on $Sp\,(2n, R)$. By the same argument $SJA \in T_S SP\,(2n, R)$ as well. Thus, the right-hand side of Eq. (22) is a vector on $Sp\,(2n, R)$, and the S dynamics will stay on the space of $Sp(2n, R)$.

We can always choose initial conditions such that S is symplectic at $t = 0$, and this will guarantee that the time-dependent transformation specified by Eq. (22) is symplectic for all t.

IV. GENERALIZED COURANT-SNYDER THEORY

We now apply the technique developed in Sec. III to the Hamiltonian system in Eq. (11). Our goal is to find a new coordinate system where the transformed Hamiltonian vanishes. This idea is identical to that in Hamilton-Jacobi theory. Applications of Hamilton-Jacobi theory include the construction of action-angle variables for periodic systems [46] and finding geodesic curves on an ellipsoid [47]. It is often required that the variables in the Hamilton-Jocabi equation can be separated in order for the technique to be effective for practical problems. This limits its application. Since our dynamics is linear, the new coordinate system can be more easily constructed using the method developed in Sec. III. We will accomplish this goal in two steps. First, we seek a coordinate transformation $\bar{z} = Sz$ such that, in the $\bar{z}$ coordinates, the Hamiltonian assumes the form

$$\bar{H} = \frac{1}{2}\bar{z}^T \bar{A}\bar{z}\,, \;\; \bar{A} = \begin{pmatrix} \mu(t) & 0 \\ 0 & \mu(t) \end{pmatrix}\,, \tag{25}$$

where $\mu(t)$ is a 2×2 matrix to be determined. To write Eq. (22) in the format of 2×2 blocks, we let

$$S = \begin{pmatrix} S_1 & S_2 \\ S_3 & S_4 \end{pmatrix},$$

and split the differential equation for S, i.e., Eq. (22), into four matrix equations,

$$\dot{S}_1 = \mu S_3 - S_1 R^T + S_2 \kappa\,, \tag{26}$$

$$\dot{S}_2 = \mu S_4 - S_1 m^{-1} + S_2 R\,, \tag{27}$$

$$\dot{S}_3 = -\mu S_1 - S_3 R^T + S_4 \kappa\,, \tag{28}$$

$$\dot{S}_4 = -\mu S_2 - S_3 m^{-1} + S_4 R\,. \tag{29}$$

Including $\mu(t)$, we have five 2×2 matrices unknown. The extra freedom is introduced by the to-be-determined $\mu(t)$. Based on the analogy with Eq. (10), we choose $S_2 \equiv 0$ to remove the freedom. We rename S_4 to be w, i.e., $w \equiv S_4$, because it will be clear later that S_4 is

the envelope matrix. Equations (26)-(29) become

$$\dot{S}_1 = \mu S_3 - S_1 R^T \,, \tag{30}$$

$$S_1 = \mu w m \,, \tag{31}$$

$$\dot{S}_3 = -\mu S_1 - S_3 R^T + w\kappa \,, \tag{32}$$

$$S_3 = -\dot{w} m + w R m, \tag{33}$$

for matrices S_1, S_3, w and μ. Because $(S_1, S_2 = 0, S_3, S_4 = w)$ describes a curve in $Sp(4)$, they are consistent with the symplectic condition $S_1 S_4^T - S_2 S_3^T = I$, i.e., $S_1 w^T = I$, which implies

$$S_1 = w^{-T} \,. \tag{34}$$

From Eq. (31), we obtain

$$\mu = \left(w m w^T \right)^{-1} . \tag{35}$$

It is straightforward to verify that Eq. (30) is equivalent to another symplectic condition $S_3 S_4^T = S_4 S_3^T$. Substituting Eqs. (32)-(35) into Eq. (32), we immediately obtain the following matrix differential equation for the envelope matrix w,

$$\frac{d}{dt}\left(\frac{dw}{dt} m - w R m \right) + \frac{dw}{dt} m R^T + w \left(\kappa - R m R^T \right) - \left(w^T w m w^T \right)^{-1} = 0 \,. \tag{36}$$

This is the desired generalized envelope equation. It generalizes the 1D envelope equation (7), or the Ermakov-Milne-Pinney equation [28–30], as well as the previous matrix envelope equation for cases with only quadrupole and skew-quadrupole magnets, i.e., $R = 0$ [21–24]. For n-degrees of freedom, the envelope matrix w will be $n \times n$, and the generalized envelope equation has the same form as Eq. (36).

Once w is solved for from the envelope equation, we can determine S_1 from Eq. (34) and S_3 from Eq. (33). In terms of the envelope matrix w, the symplectic transformation S and its inverse are given by

$$S = \begin{pmatrix} w^{-T} & 0 \\ (wR - \dot{w}) m & w \end{pmatrix} , \tag{37}$$

$$S^{-1} = \begin{pmatrix} w^T & 0 \\ (w^{-1}\dot{w} - R)\, m w^T & w^{-1} \end{pmatrix} . \tag{38}$$

The second step is to use another coordinate transformation $\bar{\bar{z}} = P(t)\bar{z}$ to transform $\bar{H}$ into a vanishing Hamiltonian $\bar{\bar{H}} \equiv 0$ at all time, thereby rendering the dynamics trivial in the new coordinates. The determining equation for the transformation $P(t)$ is

$$\dot{P} = -PJ\bar{A} = P \begin{pmatrix} 0 & -\mu \\ \mu & 0 \end{pmatrix} . \tag{39}$$

As explained in Sec. III, the P matrix satisfying Eq. (39) is symplectic because $J\bar{A} \in sp(4)$. From $\mu = \mu^T$, we know that $J\bar{A}$ is also antisymmetric, i.e., $J\bar{A}$ belongs to the Lie algebra $so(4)$ of the 4D rotation group $SO(4)$. Thus $J\bar{A} \in sp(4) \bigcap so(4)$, and $P(t)$ is a curve in the group of 4D symplectic rotations, i.e., $P(t) \in Sp(4) \bigcap SO(4) = U(2)$, provided the initial condition of $P(t)$ is chosen such that $P(0) \in Sp(4) \bigcap SO(4) = U(2)$. We call $P(t)$ the generalized phase advance, an appropriate descriptor in light of the fact that $P(t)$ is a symplectic rotation. The Lie algebra element (infinitesimal generator) $-J\bar{A} = \begin{pmatrix} 0 & -\mu \\ \mu & 0 \end{pmatrix}$ is the phase advance rate, and it is determined by the envelope matrix through Eq. (35). Since $Sp(4) \bigcap SO(4) = U(2)$, P and its inverse must have the forms

$$P = \begin{pmatrix} P_1 & P_2 \\ -P_2 & P_1 \end{pmatrix} , \tag{40}$$

$$P^{-1} = P^T = \begin{pmatrix} P_1^T & -P_2^T \\ P_2^T & P_1^T \end{pmatrix} . \tag{41}$$

Combining the two symplectic coordinate transformations, we obtain the transformation

$$\bar{\bar{z}} = G(t)z = P(t)S(t)z\,. \tag{42}$$

In the $\bar{\bar{z}}$ coordinate representation, because $\bar{\bar{H}} \equiv 0$, the dynamics is trivial, i.e., $\bar{\bar{z}} = const.$ This enables us to construct the symplectic matrix specifying the map between z_0 and $z = M(t)z_0$ as

$$M(t) = S^{-1}P^{-1}P_0S_0 = \begin{pmatrix} w^T & 0 \\ (w^{-1}\dot{w} - R)\, mw^T & w^{-1} \end{pmatrix} P^T \begin{pmatrix} w^{-T} & 0 \\ (wR - \dot{w})m & w \end{pmatrix}_0 , \tag{43}$$

where subscript "0" denotes initial conditions at $t = 0$, and P_0 is taken to be I without loss of generality. This expression for $M(t)$ generalizes the decomposition of the symplectic map for the original 1D CS theory given by Eq. (10). The first and the third matrices

in Eq. (10) obviously have the same construction as their counterparts in Eq. (43). The phase advance, as a 4D symplectic rotation P^T in Eq. (43), generalizes the 2D rotation matrix, which is also symplectic, in Eq. (10). The phase advance P is generated by its infinitesimal generator $J\bar{A}$ determined by the envelope matrix through $\mu = \left(wmw^T\right)^{-1}$. This mechanism for phase advance in 4D phase space is identical to the original 1D CS theory where the infinitesimal generator of the phase advance is w^{-2} for a scalar envelope w. The importance of the decomposition in Eqs. (43) and (10) can be appreciated from both physical and mathematical points of view. We explain the physical meaning of the decomposition here, and leave the mathematical analysis to Sec. V. The first matrix from the right is a matching transformation at $t = 0$ of the initial conditions to an equivalent focusing system, where the phase space dynamics can be characterized by a time-dependent rotation. The second matrix from the right is a transformation along the time axis in this equivalent focusing system, with the phase advance playing the role of a time-like evolution parameter. And the third matrix from the right is a back-transformation to the original coordinate system at $t > 0$.

The coordinate transformation can also be used to construct invariants of the dynamics. A general description of linear symplectic invariants can be found in Refs. [48, 49]. For any constant 4×4 positive-definite matrix ξ, the quantity

$$I_\xi = z^T S^T P^T \xi P S z \tag{44}$$

is a constant of motion, since $\bar{\bar{z}} = PSz$ is a constant of motion. The subscript "ξ" in I_ξ is used to indicate that it is an invariant associated with ξ. For the special case of $\xi = I$, the phase advance P in Eq. (44) drops out, and

$$I_{CS} \equiv z^T S^T S z = z^T \begin{pmatrix} \gamma & \alpha \\ \alpha^T & \beta \end{pmatrix} z \,, \tag{45}$$

where α, β, and γ are 2×2 matrices defined by

$$\alpha \equiv w^T S_3 \,, \tag{46}$$

$$\beta \equiv w^T w \,, \tag{47}$$

$$\gamma \equiv S_3^T S_3 + w^{-1} w^{-T} \,. \tag{48}$$

Here, we have used I_{CS} to denote this special invariant because it is the invariant that generalizes the CS invariant [1] (or Lewis invariant [31, 32]) for one degree of freedom in

Eq. (8). The matrices, α, β, and γ are the generalized Twiss parameters in higher dimensions. It is straightforward to verify that they satisfy

$$\beta\gamma = I + \alpha^2, \tag{49}$$

which is a familiar relationship in the original CS theory between the scalar Twiss parameters defined by Eqs. (4), (5) and (9). The symplectic condition $wS_3^T = S_3 w^T$ has been used in obtaining Eq. (49).

It has been demonstrated that the envelope matrix w and the invariant I_ξ define the beam dimensions and emittance for both low intensity beams and high intensity beams with strong space-charge potential [4, 5].

Note that we have "overloaded" the symbols "M, w, α, β, γ, I_{CS}" to represent the same physical quantities in both the original CS theory for one degree of freedom and the generalized CS theory in higher dimensions without causing any confusion. It is actually more appropriate to do so than not, because the quantities in higher dimensions recover their counterparts for one degree of freedom as special cases, and the correspondence between them is exact.

V. GROUP STRUCTURE OF THE GENERALIZED COURANT-SNYDER THEORY – ROTATION GAUGE AND MODIFIED IWASAWA DECOMPOSITION

In Sec. IV, we noted that initial conditions for the envelope matrix w need to satisfy the symplectic condition; otherwise they can be arbitrary. There are freedoms in the initial conditions and thus the solutions for w. But the transfer matrix M is independent from these freedoms, which are thus gauge freedoms. A subset of the gauge freedoms has the structure of the orthogonal group $O(n)$. For a time-independent element $c \in O(n)$, we define the gauge transformation $c:\ (w, P) \mapsto (\tilde{w}, \tilde{P})$ as

$$\tilde{w} = cw\,, \tag{50}$$

$$\tilde{P} = P \begin{pmatrix} c^{-1} & 0 \\ 0 & c^{-1} \end{pmatrix}. \tag{51}$$

Let's show that the transformed $\tilde{w}$ and $\tilde{P}$ also satisfy Eqs. (36) and (39), respectively, and M is gauge invariant. Multiplying Eq. (36) by c from the left to obtain the governing equation

for $\tilde{w}$,

$$\frac{d}{dt}\left(\frac{d\tilde{w}}{dt}m - \tilde{w}Rm\right) + \frac{d\tilde{w}}{dt}mR^T + \tilde{w}\left(\kappa - RmR^T\right) - \left(\tilde{w}^T\tilde{w}m\tilde{w}^T\right)^{-1} = 0\,, \tag{52}$$

which is the same as Eq. (36) with w replaced by $\tilde{w}$. According to Eq. (35), the μ matrix transforms as

$$\tilde{\mu} = c\mu c^{-1}\,.$$

Equation (39) thus can be re-expressed in the same form using $\tilde{P}$ and $\tilde{\mu}$ as

$$\frac{d}{dt}\tilde{P} = -\tilde{P}\begin{pmatrix} 0 & -\tilde{\mu} \\ \tilde{\mu} & 0 \end{pmatrix}\,. \tag{53}$$

From Eqs. (37) and (38), the S matrix and its inverse transform as

$$\tilde{S} = \begin{pmatrix} c & 0 \\ 0 & c \end{pmatrix} S\,, \tag{54}$$

$$\tilde{S}^{-1} = S^{-1}\begin{pmatrix} c^{-1} & 0 \\ 0 & c^{-1} \end{pmatrix}\,. \tag{55}$$

Combining Eqs. (50) and (51), (54) and (55), we conclude that M is invariant under the gauge transformation $c:\ (w, P) \mapsto (\tilde{w}, \tilde{P})$, i.e., $\tilde{M} = M$.

The $O(n)$ gauge group introduces an equivalent class $([w], [P])$ for the decomposition of M using (w, P). The dimension of this equivalent class is the dimension of M as a $Sp(2n)$ group. To specify S by w and $\dot{w}$, $2n^2$ numbers are needed. To specify $P \in U(n)$, additional n^2 numbers are needed. The symplectic condition for S, $S_3^T S_1 = S_1^T S_3$ brings $(n^2 - n)/2$ constrains on w and $\dot{w}$, and the $O(n)$ gauge freedom for the equivalent class is also $(n^2-n)/2$. The dimension of the decomposition is therefore

$$2n^2 + n^2 - (\frac{n^2 - n}{2} + \frac{n^2 - n}{2}) = n(2n + 1)\,, \tag{56}$$

the same as the dimension of $Sp(2n)$.

According to the polar decomposition theorem, any non-degenerate square matrix X can be uniquely factored into an orthogonal matrix O and a symmetric, positive-definite matrix Q, i.e., $X = OQ$. As a matter of fact, $Q = \sqrt{X^T X}$ and $O = XQ^{-1}$. Using this fact, at a fixed time $t = t_1$ we can always choose $c = \sqrt{w^T(t_1)w(t_1)}w^{-1}(t_1)$ such that $\tilde{w}(t_1) = cw(t_1)$

is symmetric. With this gauge, the canonical coordinate transformation at $t = t_1$ becomes

$$G = \tilde{P} \begin{pmatrix} \tilde{w}^{-1} & 0 \\ (\tilde{w}R - \dot{\tilde{w}})m & \tilde{w} \end{pmatrix}, \tag{57}$$

which is in the form of a modified Iwasawa decomposition (or pre-Iwasawa decomposition), whose importance in phase space optics [37, 38] and phase space quantum mechanics [39] have been recently realized. The modified Iwasawa decomposition is the unique decomposition of a $2n \times 2n$ symplectic matrix G in the form of

$$G = P \begin{pmatrix} L & 0 \\ QL & L^{-1} \end{pmatrix}, \tag{58}$$

where $P \in Sp(2n) \bigcap SO(2n) = U(n)$ and L is symmetric. Matrix Q is also symmetric, which is equivalent to the condition $L^T QL = (QL)^T L$ for $\begin{pmatrix} L & 0 \\ QL & L^{-1} \end{pmatrix}$ to be symplectic. These facts are also true if the decomposition is alternatively defined to be

$$G = \begin{pmatrix} L & 0 \\ QL & L^{-1} \end{pmatrix} P\,. \tag{59}$$

For a symplectic matrix, the modified Iwasawa decomposition is equivalent to the well-known Iwasawa decomposition for a semi-simple Lie group [40].

Making $\tilde{w}$ symmetric at $t = t_1$ fixes the $O(n)$ gauge because $\tilde{w}(t_1)$ is unique according to the polar decomposition theorem. However, such a choice only makes $\tilde{w}$ symmetric at $t = t_1$. As in general gauge theories, we would like to pick a gauge such that the envelope matrix is symmetric for all t. To accommodate this desired symmetry, we need to modify the governing equations, especially the envelope equation. Let

$$\begin{aligned} w(t) &= c^{-1}(t)u(t)\,, \\ u(t) &= \sqrt{\beta(t)} = \sqrt{w^T(t)w(t)}\,, \\ c^{-1}(t) &= w(t)u^{-1}(t)\,, \end{aligned}$$

be the time-dependent polar decomposition of $w(t)$. Here we use $u(t)$ to denote this special $\tilde{w}(t)$, which is symmetric and positive-definite for all t. The matrix $u(t)$ is the "symmetrized" $w(t)$ and equals the square-root of the generalized β function. We will recast the envelope equation (36) in terms of β, as in the original Courant-Snyder theory for one degree of freedom [1]. The difference is that the procedure here has to be carried out in matrix form.

Rewrite Eq. (36) as

$$\ddot{w} + \dot{w}g + wh = w^{-T}m^{-1}w^{-1}w^{-T}m^{-1}\,, \tag{60}$$

$$g \equiv (\dot{m} - Rm + mR^T)m^{-1}\,, \tag{61}$$

$$h \equiv (\kappa - RmR^T - \dot{R}m - R\dot{m})m^{-1}\,. \tag{62}$$

We symmetrize Eq. (60) by taking $w^T(\text{Eq. (60)}) + (\text{Eq. (60)})^T w$ to obtain an second order ordinary differential equation for β,

$$\ddot{\beta} - 2\dot{w}^T\dot{w} + w^T\dot{w} + g^T\dot{w}^T w + \beta h + h^T\beta = 2m^{-1}\beta^{-1}m^{-1}\,. \tag{63}$$

It is a second-order equation for β because $\dot{w}^T\dot{w}$ and $w^T\dot{w}$ can be expressed in terms of β and $\dot{\beta}$ as follows. First note that

$$\dot{w}^T\dot{w} = \dot{u}Du + \dot{u}^2 - uD^2u - uD\dot{u}\,, \tag{64}$$

$$w^T\dot{w} = uDu + u\dot{u}\,, \tag{65}$$

$$D \equiv -\dot{c}c^{-1}\,. \tag{66}$$

Both $\dot{u}$ and D in Eqs. (64) and (65) can be expressed as functions of β and $\dot{\beta}$. For $\dot{u}$, from the definition of u we obtain

$$\dot{u}u + u\dot{u} = \dot{\beta}\,, \tag{67}$$

whose left-hand side can be viewed as a linear operator on $\dot{u}$ associated with u,

$$L_u(\dot{u}) \equiv \dot{u}u + u\dot{u}\,. \tag{68}$$

The properties of the linear operator L is discussed in the Appendix. Since $u = \sqrt{\beta}$ is symmetric and positive-definite, L_u is invertible to give

$$\dot{u} = L^{-1}_{\sqrt{\beta}}(\dot{\beta})\,, \tag{69}$$

where L^{-1} is the inverse of L defined in Eq. (A.3).

To express D in terms of β and $\dot{\beta}$, we exam the symplectic condition

$$wS_3^T = S_3w^T\,, \tag{70}$$

$$S_3 \equiv -\dot{w}m + wRm\,. \tag{71}$$

Substituting in the polar decomposition $w = c^{-1}u$ gives

$$L_{umu}(D) = umuD + Dumu = (um\dot{u} - \dot{u}mu) + u(Rm - mR^T)u\,. \tag{72}$$

Therefore,

$$D = L_{umu}^{-1}\left[(um\dot{u} - \dot{u}mu) + u(Rm - mR^T)u\right]\,, \tag{73}$$

where $u = \sqrt{\beta}$ and $\dot{u} = L_u^{-1}(\dot{\beta})\,.$

Equation (63) is a second equation for β. Its solutions do not uniquely determine the envelope matrix w, which is not surprising considering that $\beta = w^T w$ is a "symmetric" version of w. However, due to the $O(n)$ gauge freedom, β contains enough information to determine the transfer map M. In terms of u and c^{-1},

$$S = \begin{pmatrix} c^{-1} & 0 \\ 0 & c^{-1} \end{pmatrix} S_u\,, \tag{74}$$

$$S_u \equiv \begin{pmatrix} u^{-1} & 0 \\ (uR - Du - \dot{u})m & u \end{pmatrix}\,. \tag{75}$$

Even though the rotation matrix $c(t)$ here is a function of t, the transformed phase advance is defined the same way as in the case of a global gauge, i.e.,

$$P_u = P\begin{pmatrix} c^{-1} & 0 \\ 0 & c^{-1} \end{pmatrix}\,. \tag{76}$$

What is modified is the governing equation for P_u,

$$\dot{P}_u = -P_u\left[\begin{pmatrix} 0 & \mu_u \\ -\mu_u & 0 \end{pmatrix} - \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}\right]\,, \tag{77}$$

$$\mu_u \equiv \left(umu^T\right)^{-1}\,. \tag{78}$$

The second term on the right-hand side of Eq. (77) is due to the dependence on t of the local gauge. At last, the canonical coordinate transformation between z and $\bar{\bar{z}}$ is

$$\bar{\bar{z}} = Gz = P_u S_u z\,, \tag{79}$$

and the transfer map is

$$M(t_0, t) = S_u^{-1} P_u^{-1} S_{u0}\,. \tag{80}$$

The symmetric decomposition furnished by Eqs. (75), (76), and (80) is equivalent to the decomposition described in Sec. IV, but it has three desirable features by comparison. The canonical coordinate transformation $P_u S_u$ in Eq. (79) has the modified Iwasawa format for all t. It comprises a curve of the modified Iwasawa decomposition, developed from a dynamical point of view. The gauge freedom is removed, and the dimension of the symplectic transfer map is directly reflected by the dimension of the decomposition. At every t, $M(t)$ is specified by two $n \times n$ symmetric matrices β and $\dot{\beta}$, and a $U(n)$ matrix P_u. The dimension of $M(t)$ is thus $(n^2+n)/2 + (n^2+n)/2 + n^2 = n(2n+1)$.

Before ending this section, we emphasize that the purpose of studying the gauge freedom is to simplify the calculation of the symplectic map M and other lattice functions and beam parameters. By investigating the gauge freedom in the matrix envelope equation for w, we have found that we can actually bypass this gauge freedom and solve for the β matrix instead, which is symmetric and does not have the gauge freedom. From Eqs. (46), (48) and (49), the generalized Twiss parameters α and γ can also be expressed in terms of β and $\dot{\beta}$. One important advantage of using the β matrix is that the symmetric matrices β and $\dot{\beta}$ form a linear space, which makes the numerical algorithms of searching for matched solutions for β much more efficient than for matched solutions for w.

VI. STABILITY ANALYSIS – SPECTRAL STABILITY AND STRUCTURAL STABILITY

The classical analysis by Courant and Snyder [1] on the instability induced by sum resonance for uncoupled transverse dynamics may give a wrong impression that coupling effects are always deleterious. The coupled dynamics can be stable or unstable depending on the specific configuration of the lattice, but certainly not more unstable than the uncoupled dynamics. The parameter space for a stable coupled lattice is probably much larger than that of a stable uncoupled lattice. In the conceptual design of the Möbius accelerator [50] and N-rolling lattice [24, 51], it was argued that strongly coupled lattice are more preferable for high-intensity beams. Strongly coupled systems have been implemented in the spiral line induction accelerator (SLIA) [52–58], which reached up to 10KA electron current at 5 MeV beam energy. Our understanding of the stability properties of coupled dynamics has been limited by the theoretical tools available. In this section, we demonstrate how the

generalized Courant-Snyder theory can be applied to study the stability of the most general focusing lattice given by Eq. (11) with weak and strong coupling components in realistic accelerators.

For a thorough understanding, it is necessary to distinguish two types of linear stability (or instability). The first type is spectral stability, which means the linear dynamics is stable for all initial perturbations. The system is spectrally unstable if there exists an initial condition that grows without bond. In most contexts, the meaning of stability is that of spectral stability. The second type is the so-called structural stability (or strong stability). It mostly applies to systems that are spectrally stable. A spectrally stable system is structurally unstable if there is a spectrally unstable system infinitesimally closed-by. Otherwise, the spectrally stable system is also structurally stable. The well-known result with respect to the stability properties of sum/difference resonances for uncoupled lattices refers to the structural stability under the influence of an infinitesimal coupling component [1].

The spectral and structural stability of the transverse dynamics in a periodic focusing lattice is determined by its one-turn (or one-period) map $M(T)$. The fact that $M(T)$ is a symplectic matrix regulates the stability properties in a significant way [41–45]. We list here the relevant results without presenting details of the proof.

The spectral property is determined by the eigenvalues and their multiplicities. There are four possibilities:

C1) All eigenvalues are distinct and on the unit circle of the complex plane.

C2) All eigenvalues are on the unit circle. There are repeated eigenvalues. But the geometric multiplicity for all eigenvalues is one.

C3) All eigenvalues are on the unit circle. There are repeated eigenvalues with multiplicity greater than one.

C4) There exits at least one eigenvalue not on the unit circle.

Cases C3 and C4 are spectrally unstable, and Cases C1 and C2 are spectrally stable. For Cases C1 and C2, we would like to know whether they are also structurally stable. It has been shown that Case C1 is structurally stable using the symplectic nature of $M(T)$ [41–45]. Case C2 needs to be sub-divided into two categories:

C2.1) For all repeated eigenvalues, the corresponding eigenvectors have the same signatures.

C2.2) There is at least one repeated eigenvalue whose eigenvectos have different signatures.

According to the Krein-Moser theorem [41–45], Case C2.1 is structurally stable and C2.2 is structurally unstable. For an eigenvector ψ of $M(T)$, its signature is defined to be the sign of its self-product $\langle\psi,\psi\rangle = \psi^* iJ\psi$. The product between two eigenvectors ψ and ϕ in general is defined to be $\langle\psi,\phi\rangle \equiv \psi^* iJ\phi$, where ψ^*denotes the complex conjugate of ψ^T.

To design a coupled lattice, it is desirable to be in Case C1, which is both spectrally and structurally stable. As mentioned previously, for the general Hamiltonian given by Eq. (11), the parameter space satisfying this condition is large enough for most applications. Given a periodic lattice, we can search for a matched solution for β, as in the original Courant-Snyder theory for one degree of freedom [1]. After a matched β is found, the one-turn map is

$$M(T) = S_0^{-1} P(T)^{-1} S_0 \,,$$

which implies that $M(T)$ is similar to $P(T)^{-1}$. Their eigenvalues and multiplicity are identical. Because $P(T)$ is a symplectic rotation, all of its eigenvalues are on the unit circle, automatically ruling out the unstable situation in C4.

The phase advance $P(T)$ also determines the structural stability of the system. To prove this assertion, let ψ and ϕ are the eigenvectors of $M(T)$. Then $S_0\psi$ and $S_0\phi$ are the eigenvectors of $P(T)^{-1}$, and

$$\langle S_0\psi, S_0\phi\rangle = \psi^* S_0^T iJ S_0\phi = \psi^* iJ\phi = \langle\psi,\phi\rangle \ , \tag{81}$$

where use had been made of the fact $S_0$is symmetric, i.e., $S_0^T J S_0 = J$. Equation (81) states that the signatures of eigenvectors of $P(T)^{-1}$ and thus its structural stability are identical to that of $M(T)$.

These analyses lead to the important conclusion that the phase advance matrix $P(T)$ completely determines both the spectral and structural stability of the general focusing lattices. This fact can significantly simplify the stability analysis in lattice design. For example, if the system is in Case C2, we only need to look at the signatures of the eigenvectors of $P(T)^{-1}$ to know if it is structurally stable. According the Krein-Moser theorem, if the

eigenvectors for all repeated eigenvalues of $P(T)^{-1}$ have the same signatures, then the system is structurally stable. Otherwise, it is structurally unstable. Let's show that this conclusion recovers the classical results on the stability properties of sum/difference resonances for uncoupled quadrupole lattices as special cases. In this case, the phase advance matrix is calculated to be [21, 22]

$$P(T)^{-1} = \begin{pmatrix} \cos\phi_x & 0 & \sin\phi_x & 0 \\ 0 & \cos\phi_y & 0 & \sin\phi_y \\ -\sin\phi_x & 0 & \cos\phi_x & 0 \\ 0 & -\sin\phi_y & 0 & \cos\phi_y \end{pmatrix},$$

where ϕ_x and ϕ_y are the one-turn phase advance in the $x-$ and $y-$directions. Its four sets of eigenvalues, eigenvectors, and signatures are

$$\lambda_{x+} = \cos\phi_x + i\sin\phi_x\,, \quad \psi_{x+} = (1,0,i,0)^T\,, \quad \sigma_{x+} = -1\,, \tag{82}$$

$$\lambda_{x-} = \cos\phi_x - i\sin\phi_x\,, \quad \psi_{x-} = (1,0,-i,0)^T\,, \quad \sigma_{x-} = 1\,, \tag{83}$$

$$\lambda_{y+} = \cos\phi_y + i\sin\phi_y\,, \quad \psi_{y+} = (0,1,0,i)^T\,, \quad \sigma_{y+} = -1\,, \tag{84}$$

$$\lambda_{y-} = \cos\phi_y - i\sin\phi_y\,, \quad \psi_{y-} = (0,1,0,-i)^T\,, \quad \sigma_{y-} = 1\,. \tag{85}$$

Resonance occurs when two or more eigenvalues collide, which has four possibilities:

R1) Self-resonance in the $x-$direction. $\phi_x = n\pi$ and $\lambda_{x+} = \lambda_{x-} = \pm 1$.

R2) Self-resonance in the $y-$direction. $\phi_y = n\pi$ and $\lambda_{y+} = \lambda_{y-} = \pm 1$.

R3) Sum resonance. $\phi_x + \phi_y = n\pi$, $\lambda_{x+} = \lambda_{y-}$ and $\lambda_{x-} = \lambda_{y+}$.

R4) Difference resonance. $\phi_x - \phi_y = n\pi$, $\lambda_{x+} = \lambda_{y+}$, and $\lambda_{x-} = \lambda_{y-}$.

Case R1 is structurally unstable because σ_{x+} and σ_{x-} are different. Case R2 is structurally unstable for the same reason.

For the sum resonance at the repeated eigenvalue $\lambda_{x+} = \lambda_{y-}$, the signatures σ_{x+} and σ_{y-} of the corresponding eigenvectors have different signs. The sum resonance is thus structurally unstable. For the difference resonance at the first repeated eigenvalue $\lambda_{x+} = \lambda_{y+}$, the corresponding eigenvectors ψ_{x+} and ψ_{y+} have the same signature. This is also true at the second repeated eigenvalue $\lambda_{x-} = \lambda_{y-}$. The difference resonance is thus structurally stable. These results are well-known previously [1], but recovered here as a special case of a more

general criterion based on the generalized phase advance and the Krein-Moser theorem [41–45]. We expect that the more general stability criterion expressed in terms of the phase advance matrix $P(T)$ to be a powerful tool for future lattice design with strong coupling.

VII. CONCLUSIONS AND FUTURE WORK

We have presented in this paper a detailed derivation of the generalized Courant-Snyder theory for the most general linear focusing lattices with quadrupole, skew-quadrupole, dipole, and solenoidal components, as well as torsion of the fiducial orbit and variation of beam energy. The theoretical structure of the theory in terms of gauge freedoms and group decomposition were described. We have also demonstrated the application of the theory in stability analysis for strongly and weakly coupled lattices. In addition to being more realistic, the most general Hamiltonian in Eq. (11) enables a much larger parameter space for designing strongly coupled lattices that are spectrally and structurally stable. The generalized Courant-Snyder parameterization scheme developed here provides an effective tool to study the coupled dynamics and to discover more optimized lattice design in the larger parameter space of general focusing lattices. The formalism also sets the theoretical foundation for investigating collective phenomena in high-intensity beams, such as the self-consistent solutions of the Vlasov-Maxwell equations in phase space including strong self-field effects that can couple the transverse dynamics [59–63].

As mentioned in Sec. IV, the theoretical framework developed is valid for linear system with any degree of freedom. In particular, we can apply it to the 3D coupled dynamics, which includes the sychrotron oscillation in RF cavities, and the linear coupling between transverse and longitudinal dynamics as in the recent investigations of emittance change [64–66]. In this case, $n = 3$ and the focusing matrix $\kappa(t)$ in Eq. (11) becomes a 3×3 matrix which describes both sychrotron and betatron oscillations as well as possible coupling between them. The envelop matrix w is 3×3 and satisfies Eq. (36) with R, m and κ being 3×3 matrices. The Twiss parameters α, β, and γ are 3×3 matrices, the symplectic matrix M is 6×6, and all the equations they satisfy are identical as in the case of 2-degrees of freedom. Studies in these directions will be reported in future publications.

Appendix: $L_x(y)$

In this Appendix, we derive the mathematical properties of the linear transformation used in Eqs. (68) and (72). Let A and X denote $n \times n$ matrices. For a symmetric, positive-definite matrix A, define the linear function associated with A on X as

$$L_A(X) \equiv AX + XA\,.$$

We prove that L_A is invertible. It is enough to show that L_A is injective, i.e., $L_A(X) = 0$ only if $X = 0$. Let X is in the kernel of L_A, i.e.,

$$L_A(X) = 0. \tag{A.1}$$

Since A is symmetric, the eigenvectors of A form a basis for vectors in R^n. Expressed in this basis, Eq. (A.1) is

$$\lambda_u v^T X u + \lambda_v v^T X u = 0\,, \tag{A.2}$$

where u and v are any pairs of vectors in the basis, and λ_u and λ_v are the corresponding eigenvalues, respectively. Because the eigenvalues of a positive-definite matrix are positive, Eq. (A.2) is possible only when $v^T X u = 0$. This proves that L_A is invertible. In terms of its components in this basis, L_A^{-1} is given as

$$u^T X v = \frac{u^T Y v}{\lambda_u + \lambda_v}\,, \tag{A.3}$$

where $Y = L_A(X)$.

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