

Symplectic tracking through curved three-dimensional fields by a method of generating functions

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Symplectic integrators play a pivotal role in the long-term tracking of charged particles within accelerators. To obtain symplectic maps in accurate simulations of single-particle trajectories, two key components are addressed: precise analytical expressions for arbitrary electromagnetic fields and a robust treatment of the equations of motion. In a source-free region, electromagnetic fields can be decomposed into harmonic functions, applicable to both scalar and vector potentials, encompassing both straight and curved reference trajectories. These harmonics are constructed according to boundary surface field data due to the uniqueness theorem. By finding generating functions to satisfy the Hamilton-Jacobi equation via a perturbative ansatz, we derive maps that are symplectic at any order of the expansion. This method yields a direct mapping from initial to final coordinates, bypassing the tracking of intermediate coordinates. Our developed particle-tracking algorithm translates the field harmonics into beam trajectories, offering a high-resolution integration method in accelerator simulations.

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I. INTRODUCTION

Accurate prediction of particle trajectories in an accelerator beamline is essential for both the design and operation of the accelerator. This is especially important for a circular machine where particles revolve for millions of turns, as the effects of any nonlinear fields or complex fringe fields are magnified. The emittance acceptance must also be carefully estimated. Accurate tracking of the exact particle path along a reference trajectory requires a precise and well-defined prior description of electromagnetic fields. Standard expressions in simple cases, like the hard-edge model, are not applicable to complex magnets. For example, novel superconducting coils or complex magnets used for an FFAG accelerator pose challenges in calculating particle trajectories [1,2]. Therefore, we need an efficient evaluation of arbitrary static electromagnetic fields before tracking. An analytical representation of the fields, which can be differentiated and integrated, is more

suitable for programming to obtain precise results for particle tracking than interpolation fitting of grid data.

For most accelerator elements, the equations of motion cannot be solved analytically and must therefore be addressed using numerical integration methods. In Hamiltonian mechanics, these equations of motion can be equivalently expressed using Hamilton's canonical equations, Poisson brackets, or the Hamilton-Jacobi equation. Symplecticity, a fundamental property of any Hamiltonian conservative system, ensures the preservation of phase-space structure and is crucial for accurate long-term particle tracking [3]. As the system described by the Hamiltonian H cannot be solved analytically, numerical integration techniques preserving symplecticity should be employed. Explicit Runge-Kutta (RK) algorithms can be applied to solve Hamilton's canonical equations to obtain particle coordinates and momenta. However, they require sufficiently small step sizes and do not inherently preserve symplecticity [4]. Poisson brackets naturally extend to a Lie algebra method, which is powerful and widely used in particle tracking [5–7]. This includes applications such as the approximation of nonseparable Hamiltonians [8] and symplectic multiparticle tracking with self-consistent space-charge simulations [9]. In Poisson bracket-based symplectic tracking, each integration step involves multiple intermediate variable transitions [6]. This reliance on the Baker-Campbell-Hausdorff (BCH) formula complicates careful code implementation.

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However, a Taylor-expanded generating function (GF) method can generate a flexible and symplectic mapping routine for particle tracking in external magnetic fields [10–13]. This method is quite general and is based on the solution of the Hamilton-Jacobi equation. The approach has been successfully used for particle tracking in straight 3D fields for accelerator-driven light sources, allowing complete parametrization and simplifying tracking studies [14]. This approach yields approximate solutions of the Hamilton-Jacobi equation, accurate to arbitrary order. However, if magnetic fields in an accelerator are configured to guide particles along a curved trajectory, such as in ring accelerators, this application of the generating function method remains unexplored. Our study aims to fill this gap by extending the generating function method to magnetic field configurations that guide particles along curved trajectories, as is common in ring accelerators. This extension is particularly valuable for synchrotrons, storage rings, and fixed-field alternating gradient (FFAG) accelerators, which often utilize complex magnet designs, including novel superconducting coils. These advanced machines present significant challenges for particle tracking due to their intricate field structures, making traditional methods less effective. By ensuring symplecticity and employing analytical field representations, our method offers a precise and efficient solution for particle trajectory prediction, which is essential for the design and operation of these sophisticated accelerator systems. To address this, a field representation that satisfies Maxwell's equations must first be established, followed by the development of an efficient method to integrate the equations of motion for particles traversing these fields. The scope of this work is limited to single-particle dynamics. Single-particle beam dynamics applies when interparticle forces are negligible—e.g., in low-current beams or high-energy sections—since space-charge forces are weak compared to external fields.

The organization of this paper is as follows: After the introduction, we present the theory of 3D descriptions for magnetic fields using harmonics, and symplectic tracking based on generating functions is discussed in Sec. II. In Sec. III, we provide the numerical results of our method and illustrate different approaches for modeling the magnetic field. Finally, conclusions are presented in Sec. IV.

II. THEORY

A. Field representation

1. 2D and axisymmetric configurations

Accurate models of electric and magnetic fields for beamline elements are essential for computing precise particle orbits and high-order transfer maps, which are critical for the performance of accelerators. In particular, for long, straight 2D accelerator magnets, field quality is efficiently characterized by a set of Fourier coefficients

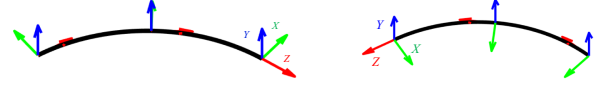


FIG. 1. The x axis (green color) of the local coordinate system is oriented away from the center of curvature for positive h (left) and toward the center for negative h (right).

a_n, b_n , known as field harmonics in the polar coordinate system, where ρ_0 is a reference radius. The longitudinal magnetic vector potential A_s is governed by the following equation:

$$A_s(\rho, \theta) = \sum_{n=1}^{\infty} \left(\frac{\rho}{\rho_0} \right)^n (a_n \sin n\theta - b_n \cos n\theta). \quad (1)$$

In a curved system characterized by curvature h , with invariance along the magnet axis and using transverse beam coordinates x and y centered on the reference trajectory, the longitudinal vector potential A_s and magnetic fields B_x, B_y are expressed as [15]:

$$\begin{aligned} \frac{\partial^2 A_s}{\partial x^2} + \frac{\partial^2 A_s}{\partial y^2} + \frac{h}{1+hx} \frac{\partial A_s}{\partial x} - \frac{h^2}{(1+hx)^2} A_s &= 0, \\ B_x &= \frac{1}{1+hx} \frac{\partial[(1+hx)A_s]}{\partial y}, \\ B_y &= \frac{-1}{1+hx} \frac{\partial[(1+hx)A_s]}{\partial x}. \end{aligned} \quad (2)$$

It is noted that the x axis of the local coordinate system is oriented away from the center of curvature for positive h and toward the center for negative h , as illustrated in Fig. 1.

Specifically, for a dipole field, a solution to Eq. (2) is expressed as

$$A_s \sim -x + \frac{hx^2}{2(1+hx)}. \quad (3)$$

Other solutions to Eq. (2) can be determined through specific analytical techniques [16]. By substituting $A_s = \frac{\mathbb{A}}{\sqrt{1+hx}}$, Eq. (2) transforms into

$$\frac{\partial^2 \mathbb{A}}{\partial x^2} + \frac{\partial^2 \mathbb{A}}{\partial y^2} = \frac{3h^2}{4(1+hx)^2} \mathbb{A}. \quad (4)$$

This transformed equation isolates the Laplace operator on the left-hand side, suggesting that preliminary approximate solutions resemble those of Eq. (1). If the curvature is small and the region of interest is within the paraxial area, the right-hand side of Eq. (4) can be neglected, and we obtain the following solution:

$$A_s \approx \frac{\rho^n e^{in\theta}}{\sqrt{1+hx}}. \quad (5)$$

To achieve higher accuracy, an iterative method substitutes this initial solution into the right-hand side of Eq. (4). The solution $\mathbb{A}$ is then refined with each iteration to progressively improve the approximation, as follows:

$$A_s = \frac{\rho^n e^{in\theta}}{\sqrt{1+hx}} \left(1 + \frac{3}{16} \frac{h^2 \rho^2}{n+1} \right). \quad (6)$$

2. 3D configurations

Whether in two dimensions or under axisymmetric conditions, these models provide simplified representations of electromagnetic field distributions, whereas the actual three-dimensional distribution is significantly more complex. In a region where no net current is enclosed by any closed loop, the magnetic field $\vec{B}$ is curl-free and can therefore be described in terms of a magnetic scalar potential ψ , such that $\vec{B} = \nabla\psi$. It must then obey the Laplace equation $\nabla^2\psi = 0$ (since $\nabla \cdot \vec{B} = 0$), which is usually solved numerically via the finite element method.

In mathematics, general solutions ψ satisfying the Laplace equation in certain orthogonal coordinate systems within a specified domain exist as analytic forms, known as harmonic functions. These magnetic field harmonics form a complete and orthogonal set in the region. Higher-order terms can be ignored, as they represent rapidly varying magnetic fields that are of minimal practical significance. Using a set of coefficients to describe the field map, both the field and its derivatives or integrals in the region of interest can be obtained by summing the contributions of the analytical field harmonics. Mathematicians have extensively studied these solutions in various specific coordinate systems, including ring [17], cylindrical [18], and spherical [19,20] domains, as illustrated in Fig. 2. Harmonics in cylindrical systems for a straight reference trajectory have been widely discussed in beam physics literature [14,18]. In this paper, we focus on harmonics in ring systems for a curved reference trajectory. Additionally, spherical

harmonics are among the most extensively studied harmonic functions, and with appropriate spherical arrangements, they can approximate any shape. This paper also explores their applications.

In accelerator physics and beam dynamics, the magnetic vector potential $\vec{A}$ is often preferred over the scalar potential ψ . Here, we choose a gauge where the longitudinal component of the vector potential is set to zero, reducing the number of variables for trajectory calculations. The scalar potential is related to the vector potential in a straight coordinate system as

$$A_x = \frac{\partial}{\partial y} \left(\int \psi dz \right), \quad A_y = -\frac{\partial}{\partial x} \left(\int \psi dz \right), \quad A_z = 0. \quad (7)$$

In a curved system, the scalar potential is related to the vector potential as

$$\begin{aligned} A_x &= (1+hx) \frac{\partial}{\partial y} \left(\int \psi ds \right), \\ A_y &= -(1+hx) \frac{\partial}{\partial x} \left(\int \psi ds \right), \\ A_s &= 0. \end{aligned} \quad (8)$$

B. Hamilton-Jacobi equations

The resolution of mechanical problems using the Hamilton-Jacobi equation adopts a systematic approach rooted in analytical mechanics. The process begins with the system's Hamiltonian, which, for a particle in an accelerator beamline, is given as [21]:

$$H = \frac{\delta}{\beta_0} - (1+hx) \times \left(a_s + \sqrt{\left(\delta + \frac{1}{\beta_0} - \frac{q\phi}{cP_0} \right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2 \gamma_0^2}} \right). \quad (9)$$

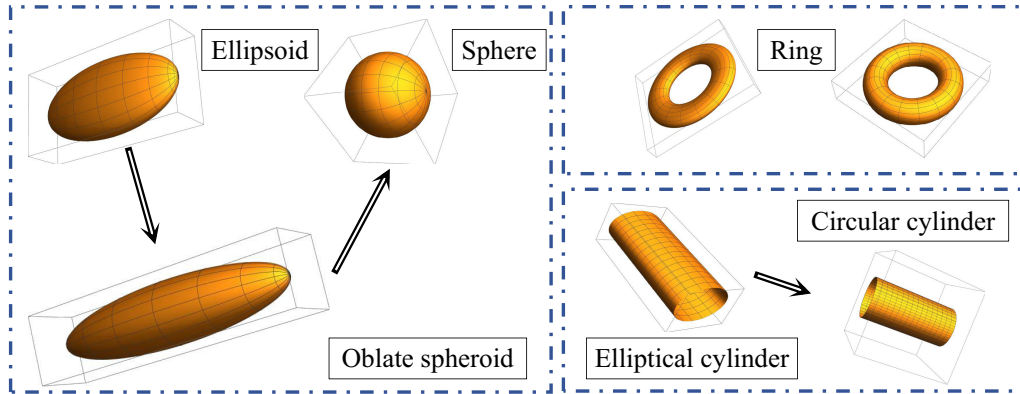


FIG. 2. Solutions to Laplace's equation in ring, cylindrical, and spherical domains are typically analyzed within their respective coordinate systems. Arrows indicate progressive symmetry specialization.

It describes the motion of a particle with energy deviation δ in an electrostatic potential ϕ and a magnetic field described by scaled vector potential components a_x, a_y, a_s (where these potentials are scaled by the reference momentum P_0). The reference particle's velocity, energy, and momentum are represented by β_0, γ_0 , and P_0 , respectively. The longitudinal coordinate s acts as a timelike parameter, while x and y are transverse coordinates with conjugate momenta p_x and p_y :

$$p_x = \frac{\gamma m_0 \beta \frac{dx}{ds} + qA_x}{P_0}, \quad p_y = \frac{\gamma m_0 \beta \frac{dy}{ds} + qA_y}{P_0},$$

$$a_x = \frac{qA_x}{P_0}, \quad a_y = \frac{qA_y}{P_0}, \quad a_s = \frac{qA_s}{P_0}. \quad (10)$$

In this paper, we consider a particle with reference energy $\delta = 0$ traversing an external magnetic field, reducing the problem to two canonical coordinates x, y and their canonical momenta p_x, p_y . We assume that the dynamical variables remain sufficiently small along the accelerator, enabling the Hamiltonian to be approximated by expanding the square root to a chosen order as follows:

$$H \approx -(1 + hx) \left[1 - \frac{1}{2}(p_x - a_x)^2 - \frac{1}{2}(p_y - a_y)^2 + a_s \right], \quad (11)$$

which serves as an effective Hamiltonian that maintains symplecticity for particle tracking under paraxial approximation in this paper.

A specific canonical transformation can be defined such that the transformed Hamiltonian becomes identically zero. The generating function F bridges the old coordinates (x, y) and momenta (p_x, p_y) with the new coordinates (u_x, u_y) and momenta (v_x, v_y) . These newly defined coordinates and momenta are constants for each particle, invariant with respect to s in the motion, though they may differ between particles. The scalar function $F(x, y, v_x, v_y)$ satisfies the first-order partial differential equation known as the Hamilton-Jacobi equation:

$$\partial_s F(x, y, v_x, v_y) = -H. \quad (12)$$

The relationship between the old and new coordinates and momenta is given by

$$p_x = \frac{\partial F}{\partial x}, \quad p_y = \frac{\partial F}{\partial y}; \quad (13a)$$

$$u_x = \frac{\partial F}{\partial v_x}, \quad u_y = \frac{\partial F}{\partial v_y}. \quad (13b)$$

By relating the original coordinates (x, y) and momenta (p_x, p_y) at both ends of a finite step (from s_0 to s_f , where

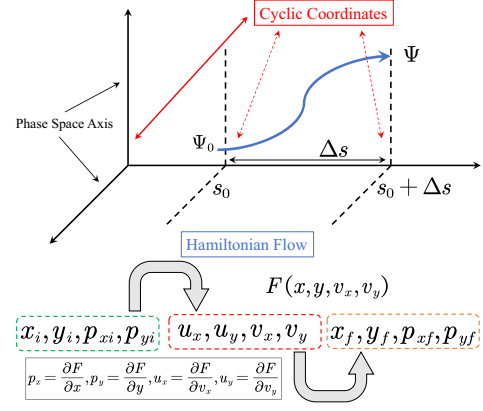


FIG. 3. Cyclic coordinates act as invariants in symplectic dynamics, linking initial and final phase-space coordinates via generating functions. The transverse axes correspond to the 4D phase space and the longitudinal axis corresponds to “time.”

the step size is $\Delta s = s_f - s_0$) to the newly defined generalized coordinates (u_x, u_y) and momenta (v_x, v_y) , this GF method calculates the motion of particles, as illustrated in Fig. 3.

By substituting Eqs. (11) and (13a) into Eq. (12), we derive the following Hamilton-Jacobi equation:

$$\partial_s F = (1 + hx) \left[1 - \frac{1}{2}(\partial_x F - \varepsilon a_x)^2 - \frac{1}{2}(\partial_y F - \varepsilon a_y)^2 + \varepsilon a_s \right], \quad (14)$$

which involves the first-order partial derivatives of F with respect to s, x, y . We introduce a parameter ε to facilitate tracking the power of the potential functions a_x, a_y , and a_s , which is ultimately set to 1, consistent with its historical use in [13,14]. We adopt a Taylor series expansion of the generating function as an ansatz, having the following form:

$$F = v_x x + v_y y + \sum_{i,j,k,l=0}^{\infty} f_{ijkl} v_x^i v_y^j h^k \varepsilon^l, \quad (15)$$

where the summation excludes the terms $f_{1000} = x$ and $f_{0100} = y$, as these are already included explicitly in the form $v_x x + v_y y$. The f_{ijkl} coefficients are functions of the local variables x, y, s , and the expansion order is given by $i + j + k + l$. By substituting Eq. (15) into Eq. (14) and considering some of the lowest-order f_{ijkl} terms, we can recursively obtain higher-order terms of f_{ijkl} . This property arises from the presence of the quadratic terms on the right-hand side of Eq. (14). The use of the parameter ε facilitates tracking the power of the potential functions a_x, a_y, a_s for the coefficients f_{ijkl} and can therefore be set to $\varepsilon = 1$ without loss of generality. It should be noted that the

introduction of the parameter ε enables the formulation of a recurrence relation for the coefficients f_{ijkl} .

Once we have determined the coefficients f_{ijkl} of the generating function, Eqs. (13a) and (13b) yield the following relationships:

$$\begin{aligned} p_x &= \sum_{i,j,k,l=0}^{\infty} \frac{\partial f_{ijkl}}{\partial x} v_x^i v_y^j h^k \varepsilon^l + v_x, \\ p_y &= \sum_{i,j,k,l=0}^{\infty} \frac{\partial f_{ijkl}}{\partial y} v_x^i v_y^j h^k \varepsilon^l + v_y. \end{aligned} \quad (16)$$

$$\begin{aligned} u_x &= \sum_{i,j,k,l=0}^{\infty} i f_{ijkl} v_x^{i-1} v_y^j h^k \varepsilon^l + x, \\ u_y &= \sum_{i,j,k,l=0}^{\infty} j f_{ijkl} v_x^i v_y^{j-1} h^k \varepsilon^l + y. \end{aligned} \quad (17)$$

The summation excludes f_{1000} and f_{0100} . If the condition $f_{ijkl}|_{s=s_f} \equiv 0$ is satisfied, then the new coordinates u_x, u_y and momenta v_x, v_y are equal to the old coordinates $x|_{s=s_f}, y|_{s=s_f}$ and momenta $p_x|_{s=s_f}, p_y|_{s=s_f}$, respectively. With a chosen expansion order for F and a small step size of $|s_0 - s_f|$, a Newton's method can be employed to solve Eq. (16) for v_x and v_y , as follows:

$$\begin{aligned} v_x &= p_x|_{s=s_0} - \sum_{i,j,k,l=0}^{\infty} \frac{\partial f_{ijkl}}{\partial x} v_x^i v_y^j h^k \varepsilon^l, \\ v_y &= p_y|_{s=s_0} - \sum_{i,j,k,l=0}^{\infty} \frac{\partial f_{ijkl}}{\partial y} v_x^i v_y^j h^k \varepsilon^l. \end{aligned} \quad (18)$$

In this process, the initial guess values for v_x and v_y can be set to $p_x|_{s=s_0}$ and $p_y|_{s=s_0}$, respectively. Typically, only a few iterations are required to converge to the solutions.

For example, in the case of no fields (the so-called ‘‘drift case’’), the Hamilton-Jacobi equation becomes

$$\partial_s F = 1 - \frac{1}{2}(\partial_x F)^2 - \frac{1}{2}(\partial_y F)^2. \quad (19)$$

The nonzero coefficients are:

$$f_{0000} = s - s_f, \quad f_{2000} = -\frac{s - s_f}{2}, \quad f_{0200} = -\frac{s - s_f}{2}. \quad (20)$$

The results from Eqs. (16) and (17) then satisfy the predictions for a drift segment:

$$\begin{aligned} p_x|_{s=s_0} &= v_x = p_x|_{s=s_f}, \\ p_y|_{s=s_0} &= v_y = p_y|_{s=s_f}, \end{aligned} \quad (21)$$

$$\begin{aligned} u_x &= x|_{s=s_f} = v_x(s_f - s_0) = p_x|_{s=s_0}(s_f - s_0), \\ u_y &= y|_{s=s_f} = v_y(s_f - s_0) = p_y|_{s=s_0}(s_f - s_0). \end{aligned} \quad (22)$$

III. TRACKING RESULTS

A. Tracking through ideal elements

1. Algorithm

In the first test, we assess the suitability of the generating function method for tracking motion through ideal hard-edge elements. We also emphasize the importance of a precise representation of the magnetic field. In nonlinear dynamical systems, accurate tracking of dynamical variables over long integration periods is paramount for a thorough understanding of their evolution.

We formalize definitions to characterize the algorithmic implementation of the recurrence relations governing the coefficients f_{ijkl} . By substituting the ansatz and performing a coefficient comparison for the Hamilton-Jacobi equation, we derive the following equations:

$$\begin{aligned} Z_{(i,j,k,l)} &= -\frac{1}{2} \sum_{\alpha=0}^i \sum_{\beta=0}^j \sum_{\gamma=0}^k \sum_{\chi=0}^l [X_{(\alpha,\beta,\gamma,\chi)} X_{(i-\alpha,j-\beta,k-\gamma,l-\chi)} \\ &\quad + Y_{(\alpha,\beta,\gamma,\chi)} Y_{(i-\alpha,j-\beta,k-\gamma,l-\chi)}] \\ &\quad - \frac{x}{2} \sum_{\alpha=0}^i \sum_{\beta=0}^j \sum_{\gamma=0}^{k-1} \sum_{\chi=0}^l [X_{(\alpha,\beta,\gamma,\chi)} X_{(i-\alpha,j-\beta,k-1-\gamma,l-\chi)} \\ &\quad + Y_{(\alpha,\beta,\gamma,\chi)} Y_{(i-\alpha,j-\beta,k-1-\gamma,l-\chi)}] \end{aligned} \quad (23)$$

where the definitions are given by

$$\begin{aligned} Z_{(i,j,k,l)} &:= f_{ijkl;s} - \delta_i^0 \delta_j^0 \delta_k^0 \delta_l^1 a_s - \delta_i^0 \delta_j^0 \delta_k^1 \delta_l^1 x a_s, \\ X_{(i,j,k,l)} &:= f_{ijkl;x} - \delta_i^0 \delta_j^0 \delta_k^0 \delta_l^1 a_x, \\ Y_{(i,j,k,l)} &:= f_{ijkl;y} - \delta_i^0 \delta_j^0 \delta_k^0 \delta_l^1 a_y. \end{aligned} \quad (24)$$

The variables X , Y , and Z are introduced to make the expressions of the Hamilton-Jacobi function more concise and manageable. The notation $f_{ijkl;\star}$ denotes the partial derivative with respect to the variable indicated by a variable $\star$. δ represents the Kronecker delta function. Higher-order f_{ijkl} terms are computed by successively differentiating lower-order terms with respect to x and y and then integrating them with respect to s .

The magnetic field for ideal hard-edge elements is derived from the solution presented in Eq. (1). In this scenario, only the potential function a_s exists, while a_x and a_y are zero. In this case, the longitudinal variable s is decoupled from the transverse variables x and y , which

allows the condition $f_{ijkl}|_{s=s_f} \equiv 0$ to be easily satisfied. Several coefficients, written out explicitly, are:

$$\begin{aligned}
 f_{0000} &= s - s_f, \quad f_{2000} = f_{0200} = -\frac{s - s_f}{2}, \quad f_{0001} = \int a_s ds, \\
 f_{1001} &= \int \left(\int \frac{\partial a_s}{\partial x} ds' \right) ds, \quad f_{0101} = \int \left(\int \frac{\partial a_s}{\partial y} ds' \right) ds, \\
 f_{0002} &= -\frac{1}{2} \int \left[\left(\int \frac{\partial a_s}{\partial x} ds' \right)^2 + \left(\int \frac{\partial a_s}{\partial y} ds' \right)^2 \right] ds, \\
 f_{0003} &= - \int (\partial_x f_{0001} \partial_x f_{0002} + \partial_y f_{0001} \partial_y f_{0002}) ds, \\
 f_{0010} &= x(s - s_f); \quad f_{2010} = f_{0210} = -\frac{x(s - s_f)}{2}; \\
 f_{0011} &= x f_{0001}; \quad f_{1011} = x f_{1001}; \quad f_{0111} = x f_{0101}; \\
 f_{0012} &= x f_{0002}; \quad f_{0013} = x f_{0003}.
 \end{aligned} \tag{25}$$

According to Eq. (6), the magnetic vector potential A_s and corresponding field components B_x, B_y for curved quadrupoles, accurate to the second order in h , are given by

$$A_s = (x^2 - y^2) + \frac{h}{2}(xy^2 - x^3) + \frac{h^2}{16}(7x^4 - 6x^2y^2 - y^4), \tag{26a}$$

$$B_x = -2y + hxy - \frac{h^2}{4}(3x^2y + y^3), \tag{26b}$$

$$B_y = -2x + \frac{h}{2}(x^2 + y^2) - \frac{h^2}{4}(x^3 + 3xy^2). \tag{26c}$$

2. Results

A beamline is used to demonstrate the significance of accurately representing the magnetic fields of curved elements. The beamline employs a combined field consisting of curved quadrupoles and dipoles with curvature $h = 1 \text{ m}^{-1}$, as illustrated in Fig. 4, which is a popular design in tumor therapy transfer systems [22]. We track a single test particle for 3000 turns within the beamline. The expansion order of f_{ijkl} is set to $i \leq 2, j \leq 2, k \leq 2, l \leq 3$, and the step length is set to $s_f - s_0 = 1 \text{ mm}$. Further increasing the expansion order does not significantly affect the results, and the relative error remains below 1×10^{-4} . We compare three different field models for the curved quadrupoles in the tracking: a linear field model, a model accurate up to the first order in h , and a model accurate up to the second order in h .

The particle trajectory over 3000 turns can be seen in Fig. 5 and is consistent with the Twiss parameter evolution shown previously. The amplitude of the transverse orbit

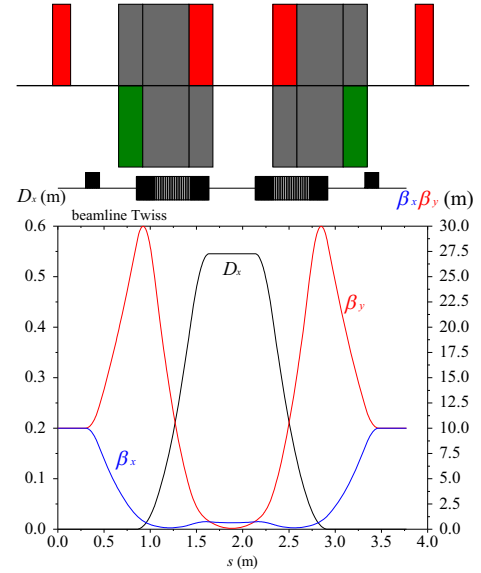


FIG. 4. Simple lattice layout with curved quadrupoles and dipoles. Top: one half of the symmetric lattice, which includes a drift, a straight focusing quadrupole, a drift, a curved defocusing quadrupole combined with a dipole, followed by another dipole, a curved focusing quadrupole combined with a dipole, and a drift, arranged sequentially. Bottom: the evolution of the Twiss parameters for this lattice, calculated using MADX.

excursion reaches 8 mm, and different field models have varying effects on long-term tracking. We record its transverse displacements at the entrance of the beamline to obtain the phase space plots shown in Fig. 6. For the different field models of curved quadrupoles, particularly when comparing the linear field model with the model incorporating the h correction, significant differences are observed in the phase space. However, the phase space characteristics of the field model with the h correction and the one with the h^2 correction appear similar. The orbit displacement as a function of turn number is Fourier transformed to determine the tunes and observe the dynamic behavior of the particle, as depicted in Fig. 7. The tunes from the linear field model deviate from those of the other two models, while the latter two exhibit

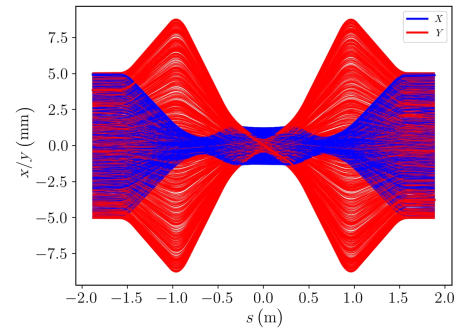


FIG. 5. Particle trajectory in the beamline for 3×10^3 turns.

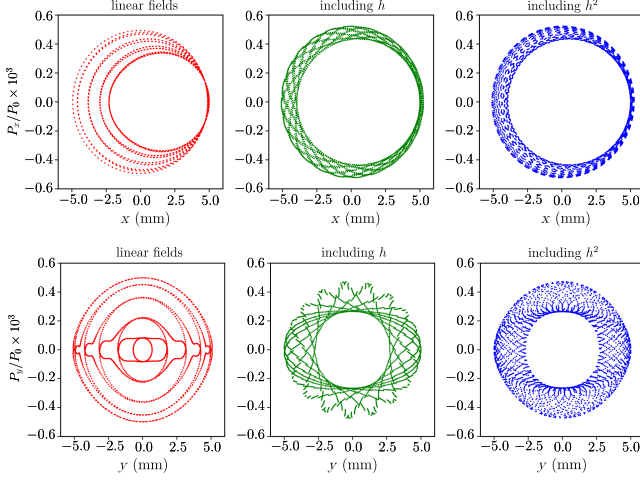


FIG. 6. Phase space of one test particle in the beamline for 3×10^3 turns. Top: $x - p_x$ phase space. Bottom: $y - p_y$ phase space. The three columns, from left to right, correspond to different field models with varying magnetic field accuracies: the linear field model, the model accurate up to the first order in h , and the model accurate up to the second order in h .

similar tunes. This demonstrates the importance of accurate field descriptions. Since the bending plane is the x axis, the difference in tune between the corrected and uncorrected cases is more pronounced in the x direction than in the y direction.

B. Tracking in bipolar coordinates

1. Bipolar coordinates

Prior work [18] models straight magnet elements (including fringe fields and multipoles) via cylindrical

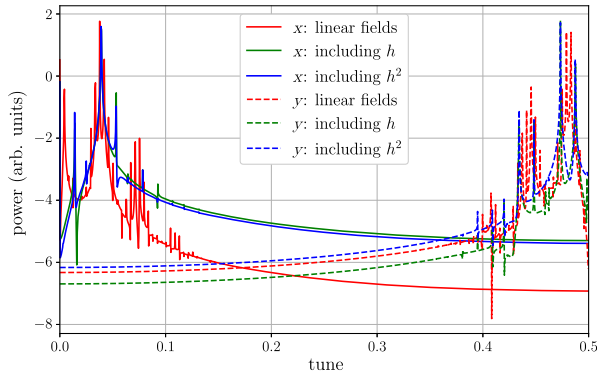


FIG. 7. Logarithmic plot of the Fourier transform of the orbit excursion over 3×10^3 turns. The peaks correspond to the tunes. Solid lines indicate the results in the x direction, while dashed lines indicate the results in the y direction. Different colors represent results from curved quadrupoles with varying magnetic field accuracies: red for the linear field model, green for the model accurate up to the first order in h , and blue for the model accurate up to the second order in h .

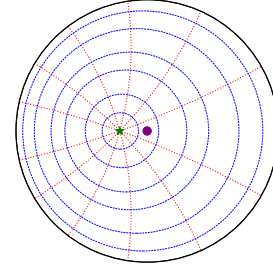


FIG. 8. In bipolar coordinates, the red curves represent lines of constant angular variable ξ ranging from 0 to 2π , while the blue curves correspond to lines of constant radial variable η within the bore surface (shown in black). Larger values of η correspond to circles of decreasing diameter, and the focus (green pentagram marker, $\eta = \infty$) for the bipolar system moves away from the center (purple circular marker, $x = 0, y = 0$) of the bore aperture.

surface data. Reference [14] then demonstrated symplectic tracking along the straight reference trajectory. Our paper focuses on magnet curved elements, which need the field representation of curved beamline elements in ring (or called “bipolar”) coordinates [23].

The coordinates in the transverse plane for curved reference trajectory inside the magnet’s bore are illustrated in Fig. 8. The bipolar coordinates η (radial) and ξ (angular) are related to x and y in the beam coordinate system by

$$\begin{aligned} \coth \frac{\eta - i\xi}{2} &= \frac{1/h + x + iy}{c}, \\ x &= \frac{c \sinh \eta}{\cosh \eta - \cos \xi} - 1/h, \\ y &= \frac{c \sin \xi}{\cosh \eta - \cos \xi}, \end{aligned} \quad (27)$$

where $h > 0$ is the central curvature of the magnet’s bore, and c is the focus in the bipolar coordinates. Here, we define a variable $k = \cosh(\eta) - \cos(\xi)$. The unit vectors $\hat{x}$, $\hat{y}$, and $\hat{s} = \hat{x} \times \hat{y}$ in the curvilinear coordinate system for particles correspond to $\hat{R}$, $\hat{Z}$, and $-\hat{\phi}$, respectively, in the cylindrical coordinate system. The ring’s axis coincides with the cylindrical coordinate system’s Z axis. We then find formulas concerning partial derivatives:

$$\begin{aligned} \left. \frac{\partial \eta}{\partial y} \right|_x &= \left. \frac{\partial \xi}{\partial x} \right|_y = -\frac{\sin \xi \sinh \eta}{c}, \\ \left. \frac{\partial \eta}{\partial x} \right|_y &= -\left. \frac{\partial \xi}{\partial y} \right|_x = -\frac{\cosh \eta \cos \xi - 1}{c}, \\ \left. \frac{\partial x}{\partial \xi} \right|_\eta &= \left. \frac{\partial y}{\partial \eta} \right|_\xi = -\frac{c \sinh \eta \sin \xi}{k^2}, \\ \left. \frac{\partial y}{\partial \xi} \right|_\eta &= -\left. \frac{\partial x}{\partial \eta} \right|_\xi = \frac{c(\cosh \eta \cos \xi - 1)}{k^2}. \end{aligned} \quad (28)$$

In terms of the bipolar coordinates, the scalar potential ψ can be written as follows [6,17,24]:

$$\begin{aligned} \nabla^2 \psi &= 0, \quad \vec{B} = \nabla \psi = \nabla \times \vec{A}, \\ \psi(\eta, \xi, \phi) &= M_{00}^\phi \phi + \sqrt{\cosh(\eta) - \cos(\xi)} \\ &\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \zeta_{m,n} \frac{Q_{|m|-\frac{1}{2}}^{[n]}[\cosh(\eta)]}{Q_{|m|-\frac{1}{2}}^{[n]}[\cosh(\eta_0)]} e^{in\phi} e^{im\xi}, \end{aligned} \quad (29)$$

where the $\zeta_{m,n}$ are coefficients representing the strength of one harmonic, η_0 is the radial bipolar coordinate for the bore, and $M_{0,0}^\phi$ represents the contribution from the net current enclosed by the curved trajectory, which is zero in this paper for simplicity. $Q_{m-\frac{1}{2}}^n(\cosh \eta)$ is the associated Legendre function of the second kind (also known as toroidal functions or ring functions), and the derivatives can be written by the recurrence relation.

$$\begin{aligned} \frac{dQ_{m-\frac{1}{2}}^n}{d\eta} &= \left(m+n-\frac{1}{2}\right) \left(m-n+\frac{1}{2}\right) Q_{m-\frac{1}{2}}^{n-1} - n \frac{Q_{m-\frac{1}{2}}^n}{\tanh \eta}, \\ \frac{dQ_{m-\frac{1}{2}}^n}{d\eta} &= \frac{m-\frac{1}{2}}{\tanh \eta} Q_{m-\frac{1}{2}}^n - \frac{m+n-\frac{1}{2}}{\sinh \eta} Q_{m-\frac{3}{2}}^n. \end{aligned} \quad (30)$$

In bipolar coordinates, the vector potential can be expressed as follows according to Eq. (8) (here, the azimuth direction $\hat{\phi}$ is opposite to that of $\hat{s}$ in a right-handed coordinate system):

$$\begin{aligned} A_\xi &= -\sinh \eta \frac{\partial}{\partial \eta} \left(\int \psi d\phi \right), \\ A_\eta &= \sinh \eta \frac{\partial}{\partial \xi} \left(\int \psi d\phi \right), \\ A_x &= -\frac{c \sinh \eta}{k} \frac{\partial}{\partial y} \left(\int \psi d\phi \right), \\ A_y &= \frac{c \sinh \eta}{k} \frac{\partial}{\partial x} \left(\int \psi d\phi \right), \\ A_\phi &= 0, A_s = 0. \end{aligned} \quad (31)$$

To illustrate the application of the generating function in bipolar coordinates, we consider a complex magnet configuration, as depicted in Fig. 9. This configuration comprises a dipole magnet (discrete-cosine-theta, DCT) with integrated quadrupole magnets (canted-cosine-thetas, CCTs) housed within each side of the bore. This integrated system provides both bending and focusing/defocusing capabilities for charged particles. The DCT dipole (45°) provides the primary bending, while the two CCT quadrupoles (200 mrad) achieve simultaneous focusing or defocusing.

For a pipe with a circular aperture of radius $r = 36$ mm and central bend radius $R = 1$ m, the focal c in bipolar

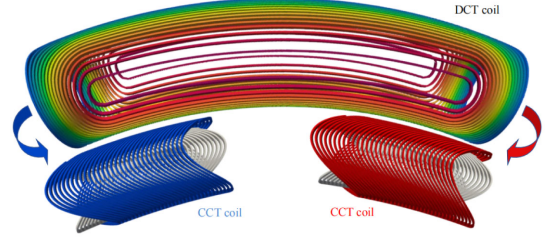


FIG. 9. Bending magnet composed of a dipole (DCT coil) with integrated quadrupoles (CCT coils) on each side of the bore provides combined bending and focusing/defocusing for charged particles. The arrows indicate that the CCT coil is positioned inside the end of the DCT coil. It is placed outside in the illustration for clarity.

coordinates and the radial coordinate parameter η_0 associated with the bore are given by

$$\begin{aligned} c &= \sqrt{R^2 - r^2}, \\ \eta_0 &= \ln \left(\frac{R + r + \sqrt{R^2 - r^2}}{R + r - \sqrt{R^2 - r^2}} \right). \end{aligned} \quad (32)$$

The normal magnetic field B_η on the surface of bore η_0 is used to obtain the bipolar coefficients $\zeta_{m,n}$. Details are provided in Appendix A [24], and the results are presented in Fig. 10. The decay of color suggests that accurately representing the magnetic field of this system necessitates retaining n to a high order, although this significantly increases the computational demands of symplectic tracking. In this work, we retain terms up to $|n| \leq 60$, $|m| \leq 16$. Ring harmonics can accurately represent real magnetic fields for curved trajectories, in principle.

The vector potential in bipolar coordinates according to Eq. (31) can be expressed as follows:

$$\begin{aligned} a_x(x, y, s) &= a_x^{(0)} s + \sum_{\substack{p=-\infty \\ p \neq 0}}^{\infty} a_x^{(p)} e^{ik_p s}, \\ a_y(x, y, s) &= a_y^{(0)} s + \sum_{\substack{p=-\infty \\ p \neq 0}}^{\infty} a_y^{(p)} e^{ik_p s}, \end{aligned} \quad (33)$$

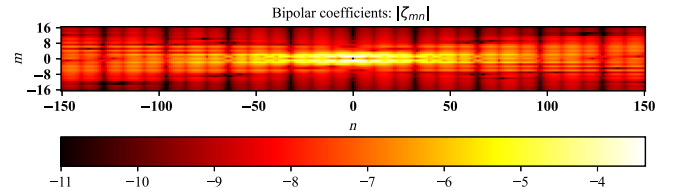


FIG. 10. Bipolar coefficients $\zeta_{m,n}$, with higher retained orders of m and n , lead to a more accurate representation of the magnetic field.

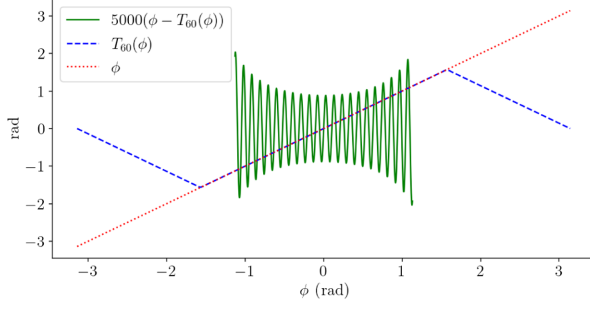


FIG. 11. Approximation of the linear function ϕ near the origin using a Fourier series. Given that the region of interest is a segment near the origin, the Fourier series of a triangular wave (in blue) is employed instead of that of a sawtooth wave (in red). Higher truncation order reduces approximation errors (green).

where $k_p = p/R$, p denotes the order of the Fourier series. To express the longitudinal position (s or ϕ) in all functions in terms of trigonometric functions, we can employ a technique to handle the linear function associated with the longitudinal coordinate. Without loss of generality, assume that ϕ is symmetric around $\phi = 0$. As the segment of interest for particle tracking is around $\phi = 0$, we consider a Fourier decomposition of triangular wave truncated at K and just use part of it, given by

$$\begin{aligned} T_K(\phi) &= \sum_{p=-K}^K \frac{g(p)}{ip} e^{ip\phi}, \\ g(p) &= 0, \quad \text{if } p = \text{even}, \\ g(p) &= 2 \frac{(-1)^{(p-1)/2}}{p\pi}, \quad \text{if } p = \text{odd}. \end{aligned} \quad (34)$$

The use of a triangular wave instead of a direct Fourier transform for ϕ is intended to facilitate faster convergence within the tracking interval, as shown in Fig. 11. As will be demonstrated later, this approximation simplifies the recurrence relationship. The vector potential can be expressed as

$$\begin{aligned} a_x(x, y, s) &= \sum_{p=-K, p \neq 0}^K \left(a_x^{(p)} + \frac{g(p)}{ip} a_x^{(0)} \right) e^{ik_p s}, \\ a_y(x, y, s) &= \sum_{p=-K, p \neq 0}^K \left(a_y^{(p)} + \frac{g(p)}{ip} a_y^{(0)} \right) e^{ik_p s}. \end{aligned} \quad (35)$$

2. Tracking codes in bipolar coordinates

We will switch back and forth between Cartesian and bipolar coordinates whenever it suits best. The Hamilton-Jacobi equation for curved reference trajectories is given by

$$\begin{aligned} \partial_s F &= (1 + hx) \left[1 - \frac{1}{2} (\partial_x F - \epsilon a_x)^2 - \frac{1}{2} (\partial_y F - \epsilon a_y)^2 \right] \\ &= (1 + hx) \left[1 - \frac{1}{2} \left(\frac{k}{c} \frac{\partial F}{\partial \eta} \Big|_{\xi, s} - \epsilon a_\eta \right)^2 \right. \\ &\quad \left. - \frac{1}{2} \left(\frac{k}{c} \frac{\partial F}{\partial \xi} \Big|_{\eta, s} - \epsilon a_\xi \right)^2 \right]. \end{aligned} \quad (36)$$

Here the longitudinal vector potential a_s vanishes due to the gauge we choose. The functions a_η and a_ξ are the corresponding normalized potentials in bipolar coordinates, and the transformation relations are expressed as follows:

$$\begin{aligned} a_\eta &= -a_x \frac{\partial y}{\partial \xi} \Big|_\eta + a_y \frac{\partial x}{\partial \xi} \Big|_\eta, \\ a_\xi &= +a_x \frac{\partial y}{\partial \eta} \Big|_\xi - a_y \frac{\partial x}{\partial \eta} \Big|_\xi, \\ a_x &= -a_\eta \frac{\partial \xi}{\partial y} \Big|_x + a_\xi \frac{\partial \eta}{\partial y} \Big|_x, \\ a_y &= +a_\eta \frac{\partial \xi}{\partial x} \Big|_y - a_\xi \frac{\partial \eta}{\partial x} \Big|_y. \end{aligned} \quad (37)$$

The momentum in bipolar coordinates is given by

$$\begin{aligned} p_\eta &= \frac{\partial F}{\partial \eta} = p_x \frac{\partial x}{\partial \eta} \Big|_\xi + p_y \frac{\partial y}{\partial \eta} \Big|_\xi, \\ p_\xi &= \frac{\partial F}{\partial \xi} = p_x \frac{\partial x}{\partial \xi} \Big|_\eta + p_y \frac{\partial y}{\partial \xi} \Big|_\eta. \end{aligned} \quad (38)$$

Here, we introduce some Fourier decomposition of $Z_{(ijkl)}$, $X_{(ijkl)}$, and $Y_{(ijkl)}$, as follows:

$$\begin{aligned} Z_{(ijkl)} &:= \frac{\partial f_{ijkl}}{\partial s} = \sum_{p=-\infty}^{\infty} \mathbb{Z}_{(ijkl)}^{(p)} e^{ik_p s}, \\ X_{(ijkl)} &:= \frac{\partial f_{ijkl}}{\partial x} - \delta_i^0 \delta_j^0 \delta_k^0 \delta_l^1 a_x = \sum_{p=-\infty}^{\infty} \mathbb{X}_{(ijkl)}^{(p)} e^{ik_p s}, \\ Y_{(ijkl)} &:= \frac{\partial f_{ijkl}}{\partial y} - \delta_i^0 \delta_j^0 \delta_k^0 \delta_l^1 a_y = \sum_{p=-\infty}^{\infty} \mathbb{Y}_{(ijkl)}^{(p)} e^{ik_p s}. \end{aligned} \quad (39)$$

The coefficient of generating function $f_{(ijkl)}$ can be reconstructed by $Z_{(ijkl)}$ as follows:

$$f_{(ijkl)} = \mathbb{Z}_{(ijkl)}^{(0)}(s - s_f) + \sum_{p=-\infty, p \neq 0}^{\infty} \frac{e^{ik_p s} - e^{ik_p s_f}}{ik_p} \mathbb{Z}_{(ijkl)}^{(p)}, \quad (40)$$

where the condition $f_{(ijkl)}|_{s_f} \equiv 0$ is satisfied automatically. Bipolar coordinates can facilitate the deduction, as the

variables are well separated and partial derivatives are simple. Here, we introduce some partial derivatives of f_{ijkl} with respect to η and ξ . Some Fourier series coefficients $\mathcal{U}$, $\mathcal{V}$ are defined as follows.

$$\begin{aligned} f_{ijkl;\eta} - \frac{c}{k} \delta_i^0 \delta_j^0 \delta_k^0 \delta_l^1 a_\eta &= \sum_{p=-\infty, p \neq 0}^{\infty} e^{ik_p s} \mathcal{U}_{(ijkl)}^{(p)}, \\ f_{ijkl;\xi} - \frac{c}{k} \delta_i^0 \delta_j^0 \delta_k^0 \delta_l^1 a_\xi &= \sum_{p=-\infty, p \neq 0}^{\infty} e^{ik_p s} \mathcal{V}_{(ijkl)}^{(p)}. \end{aligned} \quad (41)$$

For $(i, j, k, l) \neq (0, 0, 0, 1)$, the approximation of ϕ in Eq. (34) results in:

$$\begin{aligned} \mathcal{U}_{(ijkl)}^{(p)} &= \frac{\mathbb{Z}_{(ijkl)}^{(p;\eta)} + \mathbb{Z}_{(ijkl)}^{(0;\eta)} g(p)}{ik_p}, \\ \mathcal{V}_{(ijkl)}^{(p)} &= \frac{\mathbb{Z}_{(ijkl)}^{(p;\xi)} + \mathbb{Z}_{(ijkl)}^{(0;\xi)} g(p)}{ik_p}, \end{aligned} \quad p \neq 0. \quad (42)$$

We then convert back to Cartesian coordinates as follows:

$$\begin{aligned} \mathbb{X}_{(ijkl)}^{(p)} &= \frac{\partial \eta}{\partial x} \Big|_y \mathcal{U}_{(ijkl)}^{(p)} + \frac{\partial \xi}{\partial x} \Big|_y \mathcal{V}_{(ijkl)}^{(p)}, \\ \mathbb{Y}_{(ijkl)}^{(p)} &= \frac{\partial \eta}{\partial y} \Big|_x \mathcal{U}_{(ijkl)}^{(p)} + \frac{\partial \xi}{\partial y} \Big|_x \mathcal{V}_{(ijkl)}^{(p)}, \end{aligned} \quad p \neq 0. \quad (43)$$

The term corresponding to $p = 0$ is derived as follows:

$$\begin{aligned} \mathcal{U}_{(ijkl)}^{(0)} &= - \sum_{q=-\infty, q \neq 0}^{\infty} \mathcal{U}_{(ijkl)}^{(q)} e^{ik_q s_f}, \\ \mathcal{V}_{(ijkl)}^{(0)} &= - \sum_{q=-\infty, q \neq 0}^{\infty} \mathcal{V}_{(ijkl)}^{(q)} e^{ik_q s_f}, \\ \mathbb{X}_{(ijkl)}^{(0)} &= - \sum_{q=-\infty, q \neq 0}^{\infty} \mathbb{X}_{(ijkl)}^{(q)} e^{ik_q s_f}, \\ \mathbb{Y}_{(ijkl)}^{(0)} &= - \sum_{q=-\infty, q \neq 0}^{\infty} \mathbb{Y}_{(ijkl)}^{(q)} e^{ik_q s_f}, \end{aligned} \quad p = 0. \quad (44)$$

We obtain the recurrence relation for high-order coefficients of generating functions:

$$\begin{aligned} \mathbb{Z}_{(ijkl)}^{(p)} &= - \frac{1}{2} \frac{k^2}{c^2} \sum_{\alpha\beta\gamma\chi, q} \left[\mathcal{U}_{(\alpha\beta\gamma\chi)}^{(q)} \mathcal{U}_{(i-\alpha, j-\beta, k-\gamma, l-\chi)}^{(p-q)} \right. \\ &\quad \left. + \mathcal{V}_{(\alpha\beta\gamma\chi)}^{(q)} \mathcal{V}_{(i-\alpha, j-\beta, k-\gamma, l-\chi)}^{(p-q)} \right] \\ &\quad - \frac{x}{2} \frac{k^2}{c^2} \sum_{\alpha\beta\gamma\chi, q} \left[\mathcal{U}_{(\alpha\beta\gamma\chi)}^{(q)} \mathcal{U}_{(i-\alpha, j-\beta, k-1-\gamma, l-\chi)}^{(p-q)} \right. \\ &\quad \left. + \mathcal{V}_{(\alpha\beta\gamma\chi)}^{(q)} \mathcal{V}_{(i-\alpha, j-\beta, k-1-\gamma, l-\chi)}^{(p-q)} \right]. \end{aligned} \quad (46)$$

Finally, we calculate the coordinates and momentum at the end of the stepping.

$$\begin{aligned} p_{xf} &= - \sum_{ijkl} (p_{xf})^i (p_{yf})^j h^k \epsilon^l \left[\mathbb{Z}_{(ijkl)}^{(0;x)} (s - s_f) \right. \\ &\quad \left. + \sum_{p=-\infty, p \neq 0}^{\infty} \mathbb{Z}_{(ijkl)}^{(p;x)} \frac{e^{ips_0} - e^{ips_f}}{ip} \right] + p_{x0}, \\ p_{yf} &= - \sum_{ijkl} (p_{xf})^i (p_{yf})^j h^k \epsilon^l \left[\mathbb{Z}_{(ijkl)}^{(0;y)} (s - s_f) \right. \\ &\quad \left. + \sum_{p=-\infty, p \neq 0}^{\infty} \mathbb{Z}_{(ijkl)}^{(p;y)} \frac{e^{ips_0} - e^{ips_f}}{ip} \right] + p_{y0}. \end{aligned} \quad (47)$$

$$\begin{aligned} x_f &= \sum_{ijkl} i (p_{xf})^{i-1} (p_{yf})^j h^k \epsilon^l \left[\mathbb{Z}_{(ijkl)}^{(0)} (s_0 - s_f) \right. \\ &\quad \left. + \sum_{p=-\infty, p \neq 0}^{\infty} \mathbb{Z}_{(ijkl)}^{(p)} \frac{e^{ips_0} - e^{ips_f}}{ip} \right] + x_0, \\ y_f &= \sum_{ijkl} j (p_{xf})^i (p_{yf})^{j-1} h^k \epsilon^l \left[\mathbb{Z}_{(ijkl)}^{(0)} (s_0 - s_f) \right. \\ &\quad \left. + \sum_{p=-\infty, p \neq 0}^{\infty} \mathbb{Z}_{(ijkl)}^{(p)} \frac{e^{ips_0} - e^{ips_f}}{ip} \right] + y_0. \end{aligned} \quad (48)$$

The algorithm described above can be implemented through code. We track 36 particles initially uniformly distributed within a circle of radius 5 mm, observing their motion in the curved beamline shown in Fig. 9. The results are presented in Fig. 12, aligning with our expectations for the beamline field settings. The GF method is truncated at the order $i + j + k + l \leq 2$. Attempts to use higher-order truncations result in a substantial increase in memory requirements, making further calculations infeasible. At the end of the beamline, we analyze the tracking results for different step sizes, $ds=10, 5, 2.5$ mm and compare them with the fine-step (0.5 mm) Runge-Kutta tracking results,

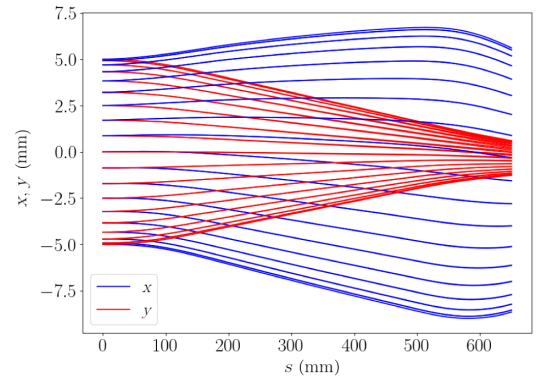


FIG. 12. Symplectic tracking of particles in bipolar coordinates by generating function. The order of field harmonics is truncated to $|n| \leq 60$ in generating function.

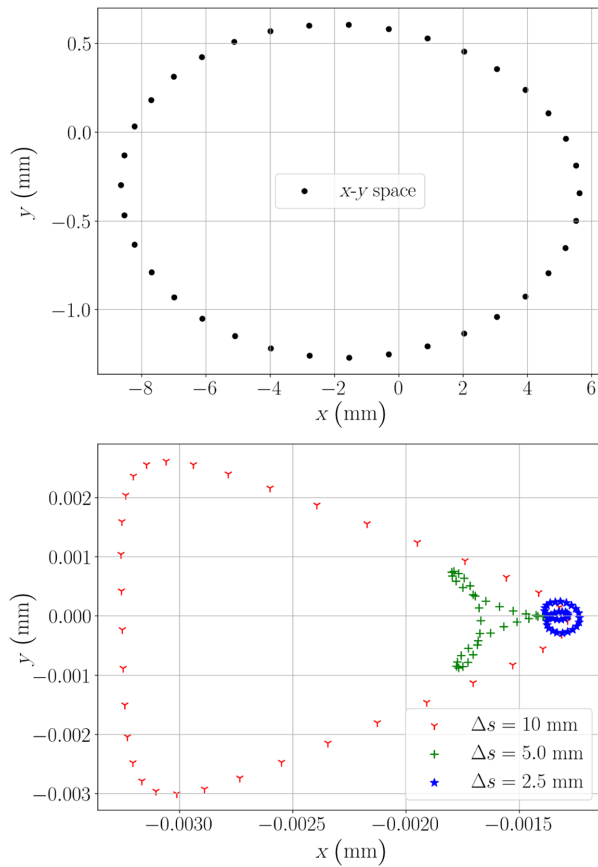


FIG. 13. Tracking results in ring coordinates at the end of the beamline are shown ($i + j + k + l \leq 2$). Three different step sizes are used for tracking through the beamline: red (10 mm), green (5 mm), and blue (2.5 mm). In the upper figure, black points represent the results in the $x - y$ phase space. In the lower figure, the three types of points denote the difference between the GF and RK methods.

as shown in Fig. 13. The error is below 0.1% relatively. Overall, the error remains small and decreases as the step size is reduced. Due to the Fourier expansion approximation of s and the finite expansion series of the generating function, the center of the error deviates from the origin even if the step size is small. In general, for sufficiently ample computational resources and with high enough truncation of the expansion series in F , symplectic tracking based on ring coordinates is feasible. However, this approach is not practical on typical desktop computers.

Cylindrical coordinates are particularly well suited for modeling straight beamlines, whereas ring coordinates are more appropriate for curved beamlines. At the junctions where straight and curved reference trajectories meet, the superposition of magnetic fields from both sides necessitates a transition to spherical coordinates to accurately account for the field complexity, as depicted in Fig. 14. It is important to note that transitioning between different coordinate systems for particles requires a conversion between canonical and mechanical

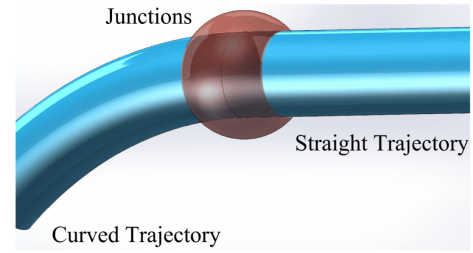


FIG. 14. Beamline comprises both straight and curved segments. Cylindrical coordinates are applicable in the straight segments, while ring coordinates are more suitable for the curved segments. Spherical coordinates can be employed at the junctions due to the complex superposition of fields from two sides.

momentum. Although this configuration can be used to track particles in any beamline, the approximation of longitudinal position through Fourier decomposition may introduce errors over long-term tracking. Additionally, the high-order expansion of the generating function demands substantial computational resources, as the field representation in both cylindrical and ring coordinates involves numerous terms. In the following subsection, we will introduce an alternative method.

C. Tracking through a series of spheres

1. Spherical coordinates

The uniqueness theorem in electromagnetism states that if the normal component of the magnetic field B_n is known on a closed surface within a source-free region, then the magnetic field inside is uniquely determined. Furthermore, the two fundamental sources that generate magnetic fields are magnetic moments, which correspond to current loops and can also be interpreted as magnetic dipoles and hypothetical magnetic monopoles. We can artificially place magnetic moments or monopoles externally, outside the region of interest, to achieve the same normal magnetic field boundary conditions B_n (called Neumann boundary condition) on the surface of the region used for tracking, thereby enabling the reconstruction of the magnetic field within the surface. The magnetic field generated by both magnetic dipoles and monopoles can be expressed in terms of spherical harmonics, as detailed in Appendix B. One key advantage of this representation is its expressibility in Cartesian coordinates transformed from spherical coordinates. For a beamline composed of straight and curved segments connected in series, a sequence of spherical elements can be used to model such a beamline. Each sphere in this sequence corresponds to a local Cartesian coordinate system. Within each sphere, local magnetic field information is encoded using spherical harmonics calculated from the reconstructed sources, as seen in Fig. 15 [25,26].

The beamline shown in Fig. 9 consists of curved segments and extended straight sections. The particles

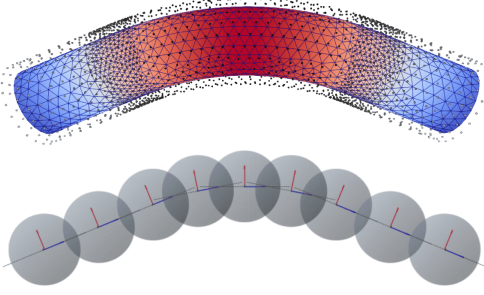


FIG. 15. By placing magnetic moments or monopoles externally (represented as the surrounding dots), outside the pipe, to satisfy the specified normal magnetic field boundary conditions B_n on its surface, the magnetic field within the surface is uniquely determined. The reconstructed field is stored in a series of spheres, each with its own Cartesian coordinate system. As particles move, their coordinate system and sphere index should be adjusted accordingly. Arbitrary beamlines can be simulated through the assembly of multiple spheres.

primarily experience the curved beamline. At the entrance and exit of the beamline, they also traverse extended straight sections. Magnetic dipoles are employed to reconstruct the magnetic fields, and the details of the procedure are shown in [27]. The strength of the field harmonics used to represent the scalar potential in a sphere along the beamline is illustrated in Fig. 16. The vector potential can be computed using the relation in Eq. (7). High-order harmonics can be neglected in the field representation due to the rapid decay of the strength. The advantage of this approach is the high precision of magnetic field reconstruction, allowing for an analytical representation of the local magnetic field, including the magnetic vector potential and magnetic scalar potential. The disadvantage is that, as the beam moves, it is necessary to switch between different spherical coordinate systems based on its position.

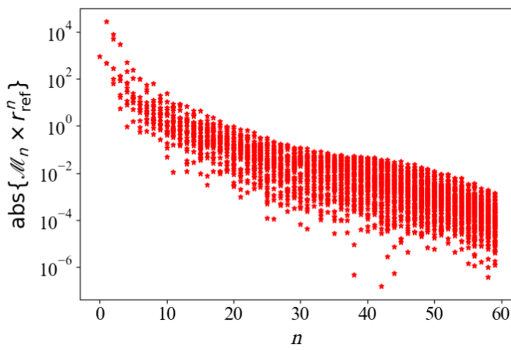


FIG. 16. The y axis represents the spherical harmonic coefficients in one sphere along the beamline, scaled by r_{ref}^n to ensure consistent units and comparable intensity. The strength of the field harmonics decreases rapidly with increasing order of spherical harmonics, and very high-order harmonics can be neglected for field map.

The particle's momentum switches between canonical and mechanical momentum.

2. Tracking codes in spherical coordinates

The Hamilton-Jacobi equation becomes simpler within spherical regions that are described by Cartesian fields, as opposed to curved coordinates, due to a reduction in the degrees of freedom. The simplified form of the equation is given by

$$\partial_z F = 1 - \frac{1}{2}(\partial_x F - \epsilon a_x)^2 - \frac{1}{2}(\partial_y F - \epsilon a_y)^2. \quad (49)$$

The longitudinal coordinate is represented within the coefficients of the generating function by means of Taylor series rather than trigonometric functions in the original paper [14]. The coefficients $f_{(ijl)}$ in the generating function can be decomposed as follows:

$$\begin{aligned} Z_{(ijl)} &:= \frac{\partial f_{(ijl)}}{\partial z} = \sum_{p=0}^{\infty} \mathbb{Z}_{(ijl)}^{(p)} z^p, \\ f_{(ijl)} &= \sum_{p=1}^{\infty} \mathbb{Z}_{(ijl)}^{(p-1)} \frac{z^p - z_f^p}{p}. \end{aligned} \quad (50)$$

The derivatives of $f_{(ijl)}$ with respect to x, y are represented as follows:

$$\begin{aligned} X_{(ijl)} &:= \frac{\partial f_{(ijl)}}{\partial x} - \delta_i^0 \delta_j^0 \delta_l^1 a_x = \sum_{p=0}^{\infty} \mathbb{X}_{(ijl)}^{(p)} z^p, \\ Y_{(ijl)} &:= \frac{\partial f_{(ijl)}}{\partial y} - \delta_i^0 \delta_j^0 \delta_l^1 a_y = \sum_{p=0}^{\infty} \mathbb{Y}_{(ijl)}^{(p)} z^p. \end{aligned} \quad (51)$$

For $(i, j, l) \neq (0, 0, 1)$, we have:

$$\mathbb{X}_{(ijl)}^{(p)} = \begin{cases} \frac{\mathbb{Z}_{(ijl)}^{(p-1;x)}}{p}, & \text{if } p > 0; \\ -\sum_{q=1}^{\infty} \mathbb{X}_{(ijl)}^{(q)} z_f^q, & \text{if } p = 0. \end{cases} \quad (52)$$

$$\mathbb{Y}_{(ijl)}^{(p)} = \begin{cases} \frac{\mathbb{Z}_{(ijl)}^{(p-1;y)}}{p}, & \text{if } p > 0; \\ -\sum_{q=1}^{\infty} \mathbb{Y}_{(ijl)}^{(q)} z_f^q, & \text{if } p = 0. \end{cases} \quad (53)$$

The recurrence relation for high-order coefficients is given by

$$\begin{aligned} \mathbb{Z}_{(ijl)}^{(p)} &= -\frac{1}{2} \sum_{(\alpha, \beta, \chi)} \sum_{q=0}^p \left[\mathbb{X}_{(\alpha, \beta, \chi)}^{(q)} \mathbb{X}_{(i-\alpha, j-\beta, l-\chi)}^{(p-q)} \right. \\ &\quad \left. + \mathbb{Y}_{(\alpha, \beta, \chi)}^{(q)} \mathbb{Y}_{(i-\alpha, j-\beta, l-\chi)}^{(p-q)} \right]. \end{aligned} \quad (54)$$

The Newton's method to obtain the final momentum is given by

$$\begin{aligned} p_{xf} &= p_{x0} - \sum_{ijl} \left[\left(\sum_{p=1}^{\infty} \mathbb{Z}_{(ijl)}^{(p-1;x)} \frac{z_0^p - z_f^p}{p} \right) (p_{xf})^i (p_{yf})^j \epsilon^l \right], \\ p_{yf} &= p_{y0} - \sum_{ijl} \left[\left(\sum_{p=1}^{\infty} \mathbb{Z}_{(ijl)}^{(p-1;y)} \frac{z_0^p - z_f^p}{p} \right) (p_{xf})^i (p_{yf})^j \epsilon^l \right]. \end{aligned} \quad (55)$$

Then the final coordinate is derived:

$$\begin{aligned} x_f &= \sum_{ijl} \left(\sum_{p=1}^{\infty} \mathbb{Z}_{(ijl)}^{(p-1)} \frac{z_0^p - z_f^p}{p} \right) i (p_{xf})^{i-1} (p_{yf})^j \epsilon^l + x_0, \\ y_f &= \sum_{ijl} \left(\sum_{p=1}^{\infty} \mathbb{Z}_{(ijl)}^{(p-1)} \frac{z_0^p - z_f^p}{p} \right) j (p_{xf})^i (p_{yf})^{j-1} \epsilon^l + y_0. \end{aligned} \quad (56)$$

The spherical harmonics used to represent the field are truncated at order $p \leq 50$ to ensure precise reconstruction of the field. We track 36 particles initially uniformly distributed within a circle of radius 5 mm in the beamline (including both straight and curved segments), and the results are presented in Fig. 17. Figures 12 and 17 are not directly comparable. In Fig. 12, particles only experience the curved beamline. Whereas in Fig. 17, they also pass through extended straight sections at the entrance and exit. At the end of the beamline, we analyze the tracking results for different settings, including varied step sizes ds and truncated orders for the generating function $i + j + l$, and compare them with the fine-step (0.5 mm) Runge-Kutta tracking results, as shown in Fig. 18. The error is below 0.02% relatively. Overall, the error is very small. Even with a step size as large as 10 mm, truncating the order to $i + j + l \leq 3$ still yields excellent tracking results. The

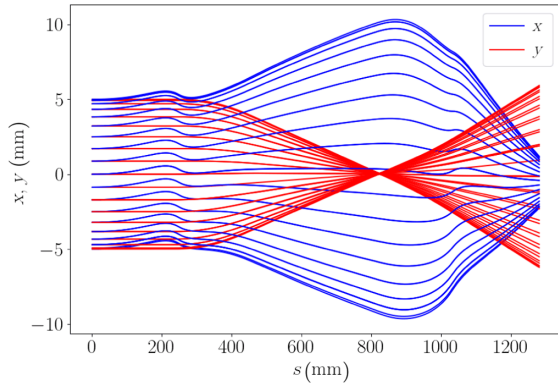


FIG. 17. Symplectic tracking of particles in spherical coordinates by generating function.

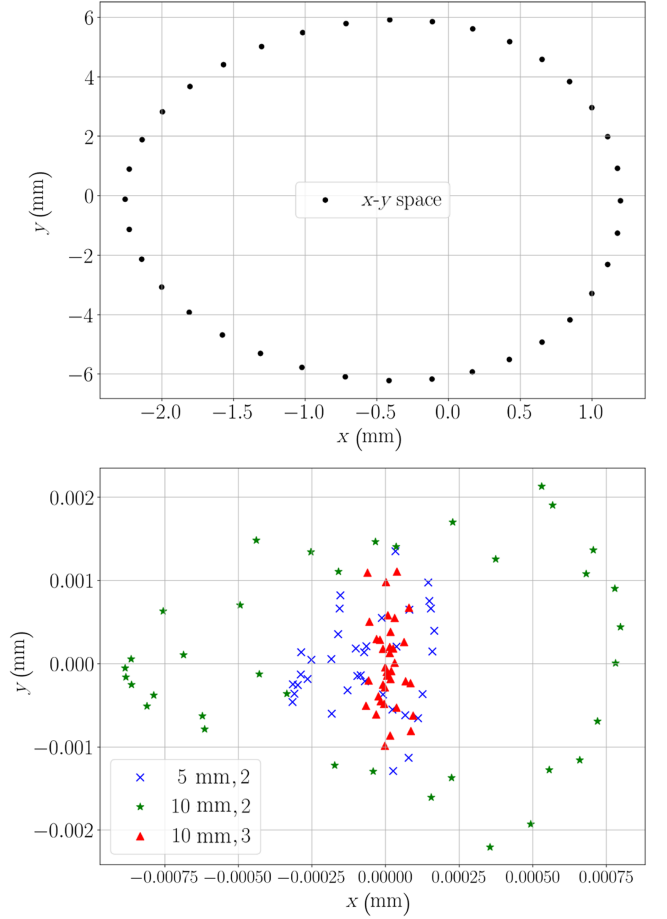


FIG. 18. Tracking results in spherical coordinates at the end of the beamline are shown. Three different settings for the GF method are used for tracking through the beamline: blue ($ds = 5$ mm, order truncated to $i + j + l \leq 2$), green ($ds = 10$ mm, order truncated to $i + j + l \leq 2$), and red ($ds = 10$ mm, order truncated to $i + j + l \leq 3$). In the upper figure, the black point represents the results in the $x - y$ phase space. In the lower figure, three types of points denote the difference between the GF and RK methods.

code is tested on a laptop with an Intel(R) Core(TM) i7-9750H CPU @ 2.60 GHz using Python for orders up to 3.

IV. CONCLUSION

We introduce a tracking scheme based on the generating function for curved magnetic elements. The field description is detailed under axisymmetric conditions or through 3D harmonic expansions. The Hamilton-Jacobi equation is solved using the perturbation method. Several tests have been conducted to validate the algorithm, including hard-edge magnets under axisymmetric conditions, curved magnets with a reference orbit described by toroidal (ring) functions, and multisphere models for any beamline.

It is noted that the accuracy of this calculation is dependent on the orders of expansion for generating function F , and, in principle, can be enhanced to achieve

arbitrary precision given sufficient computational resources. The new method is expected to be extremely useful for beamlines with special magnet designs, such as those employed in proton therapy with compact superconducting magnets or in intricate field configurations within ring accelerators.

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DATA AVAILABILITY

The data are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: FIELD REPRESENTATION IN CYLINDRICAL COORDINATES

The two referenced papers, [18,24], describe the procedure for extracting the relevant field representation coefficients for harmonic functions using cylindrical or ring surface data. For both straight and curved beamline elements, a multipole decomposition approach, based on fitting numerical data to a bounding surface, ensures a significant reduction of residuals within the bounded region.

Within an infinitely extended straight cylindrical geometry, the magnetic scalar potential can be expressed as

$$\psi(\rho, \theta, z) = \sum_{m \geq 0} \int_{-\infty}^{\infty} dk \times \psi^{(m)}(k) I_m(k\rho) e^{im\theta} e^{ikz}, \quad (\text{A1})$$

where $I_m(k\rho)$ means the modified Bessel function [28]. For a cylindrical geometry with longitudinal periodicity L , the magnetic scalar potential is expressed as follows:

$$\begin{aligned} \psi(\rho, \theta, z) = & \sum_{m \geq 0} \psi^{(m,0)} \rho^m e^{im\theta} \\ & + \sum_{m \geq 0} \sum_{k \neq 0} \psi^{(m,k)} I_m\left(k \frac{2\pi}{L} \rho\right) e^{im\theta} e^{ik \frac{2\pi}{L} z}. \end{aligned} \quad (\text{A2})$$

The radial magnetic field on the cylindrical surface is calculated as follows:

$$\begin{aligned} B_\rho = & \sum_{m \geq 0} \psi^{(m,0)} m \rho^{m-1} e^{im\theta} \\ & + \sum_{m \geq 0} \sum_{k \neq 0} \psi^{(m,k)} \frac{\partial I_m}{\partial \rho} e^{im\theta} e^{ik \frac{2\pi}{L} z}. \end{aligned} \quad (\text{A3})$$

In the magnet simulation software, the coefficients $\psi^{(m,k)}$ can be derived from B_ρ by performing two-dimensional Fourier transforms separately with respect to θ and z .

Similarly, the “radial” magnetic field B_η on the bore surface of a ring geometry is given by

$$\begin{aligned} B_\eta(\eta_0, \xi, \phi) = & \frac{k^{\frac{3}{2}}}{c} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \zeta_{m,n} e^{in\phi} e^{im\xi} \\ & \times \left\{ \frac{\sinh(\eta_0)}{2k} + \frac{\frac{\partial}{\partial \eta} Q_{|m|-\frac{1}{2}}^{[n]} [\cosh(\eta_0)]}{Q_{|m|-\frac{1}{2}}^{[n]} [\cosh(\eta_0)]} \right\}. \end{aligned} \quad (\text{A4})$$

Here, the “angle” variable ξ is not well separated in the expression. To determine the coefficients $\zeta_{m,n}$, we employ a simple analytical approach. The Fourier decomposition on the ring surface η_0 with respect to the geometric angle θ is straightforward to derive. Concurrently, the Fourier decomposition of each ring in terms of θ can also be numerically obtained. By establishing a comparative framework between these two decompositions, we formulate a matrix equation that uniquely determines the coefficients $\zeta_{m,n}$.

APPENDIX B: FIELD GENERATED BY THE MAGNETIC MOMENTS

The Helmholtz theorem states that the inner fields can be reconstructed by the magnetic field on the surface of the region [29]:

$$\begin{aligned} \vec{B}(\vec{x}) = & \nabla \times \vec{A}_t(\vec{x}) + \nabla \varphi_n(\vec{x}), \\ \varphi_n(\vec{x}) = & \frac{1}{4\pi} \int_{\partial\Omega} \frac{\vec{n}(\vec{x}_s) \cdot \vec{B}(\vec{x}_s)}{|\vec{x} - \vec{x}_s|} ds, \\ \vec{A}_t(\vec{x}) = & -\frac{1}{4\pi} \int_{\partial\Omega} \frac{\vec{n}(\vec{x}_s) \times \vec{B}(\vec{x}_s)}{|\vec{x} - \vec{x}_s|} ds. \end{aligned} \quad (\text{B1})$$

Moreover, the uniqueness theorem in electrodynamics posits that the normal component of the magnetic field B_n on the boundary surface of the region is sufficient to uniquely determine and reconstruct the internal magnetic field. If the magnetic moments or monopoles outside the region are appropriately configured to satisfy the B_n boundary condition, the internal magnetic field can be accurately reconstructed.

Considering a cluster of current elements $I_j d\vec{l}_j$ with spherical coordinates (r_j, θ_j, ϕ_j) far away from the origin, the vector potential at the origin can be calculated by the Biot-Savart law as follows:

$$\begin{aligned} \vec{A}(r, \theta, \phi) = & \mu_0 \sum_{n=0}^{\infty} \sum_{m=-n}^n \vec{M}_{n,m} \times r^n Y_{n,m}(\theta, \phi), \\ \vec{M}_{n,m} = & \sum_j \frac{I_j d\vec{l}_j}{2n+1} \frac{Y_{n,m}(\theta_j, \phi_j)}{r_j^{n+1}}. \end{aligned} \quad (\text{B2})$$

The magnetic moment can be defined as the limit of a current loop. The coefficient $\vec{M}_{n,m}$ for a magnetic moment located at (r_0, θ_0, ϕ_0) with direction (Θ, Φ) is calculated as follows:

$$\begin{aligned} \vec{M}_{n,m} = & \frac{|\vec{m}|(n+1)}{r_0^{n+2}(2n+1)} Y_{n,m}(\hat{r}_0 \times \hat{m}) \\ & + \frac{|\vec{m}|}{r_0^{n+2}(2n+1)} \frac{\partial Y_{n,m}}{\partial \cos \theta} \left(-\hat{z} \times \hat{m} - \frac{z_0}{r_0} \hat{m} \times \hat{r}_0 \right) \\ & + \frac{|\vec{m}|}{r_0^{n+2}(2n+1)} \frac{\partial Y_{n,m}}{\partial \phi} \left[\frac{\cos \Theta \sin(\Phi - \phi_0)}{\sin \theta_0} \frac{\hat{z} \times \hat{m}}{|\hat{z} \times \hat{m}|} \right. \\ & \left. - \frac{\cos(\Phi - \phi_0)}{\sin \theta_0} \frac{(\hat{z} \cdot \hat{m})\hat{m} - \hat{z}}{|\hat{z} \times \vec{m}|} \right]. \end{aligned} \quad (\text{B3})$$

Specifically, if the magnetic moment is located at the polar axis $\theta_0 = 0, \pi$, the only nonzero coefficients $\vec{M}_{n,m}$ are given by

$$\begin{aligned} \vec{M}_n^{-1} &= -\cos^{n+1} \theta_0 \frac{-m_x \hat{e}_z + m_z \hat{e}_x}{2n+1} \frac{K_n^1}{r_0^{n+2}} \frac{n(n+1)}{\sqrt{2}}, \\ \vec{M}_n^0 &= \cos^{n+1} \theta_0 \frac{m_x \hat{e}_y - m_y \hat{e}_x}{2n+1} \frac{(n+1)K_n^0}{r_0^{n+2}}, \\ \vec{M}_n^1 &= -\cos^{n+1} \theta_0 \frac{m_y \hat{e}_z - m_z \hat{e}_y}{2n+1} \frac{K_n^1}{r_0^{n+2}} \frac{n(n+1)}{\sqrt{2}}. \end{aligned} \quad (\text{B4})$$

The scalar potential of a magnetic moment can be represented by spherical harmonics as follows:

$$\begin{aligned} \varphi &= \mu_0 \sum_{n=0}^{\infty} \sum_{m=-n}^n r^n Y_{n,m}(\theta, \phi) \mathcal{M}_{n,m}, \\ \mathcal{M}_{n,m} &= \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{|\vec{m}|}{(2n+1)r_0^{n+2}} \left[(n+1) \hat{r}_0 \cdot \hat{m} Y_{n,m} \right. \\ & \quad \left. + \frac{\partial Y_{n,m}}{\partial \cos \theta} \left(\frac{z_0}{r_0} \hat{r}_0 \cdot \hat{m} - \cos \Theta \right) - \frac{\partial Y_{n,m}}{\partial \phi} \frac{\hat{z} \cdot (\hat{r}_0 \times \hat{m})}{(\hat{r}_0 \times \hat{z})^2} \right]. \end{aligned} \quad (\text{B5})$$

Specifically, if the magnetic moment is located at the polar axis $\theta_0 = 0, \pi$, the only nonzero coefficients $\mathcal{M}_{n,m}$ are given by

$$\begin{aligned} \mathcal{M}_{n,-1} &= -\cos^{n+1} \theta_0 \frac{K_n^1 m_y}{\sqrt{2}(2n+1)} \frac{(n+1)n}{r_0^{n+2}}, \\ \mathcal{M}_{n,0} &= \cos^{n+1} \theta_0 \frac{K_n^0 m_z}{2n+1} \frac{n+1}{r_0^{n+2}}, \\ \mathcal{M}_{n,1} &= -\cos^{n+1} \theta_0 \frac{K_n^1 m_x}{\sqrt{2}(2n+1)} \frac{(n+1)n}{r_0^{n+2}}. \end{aligned} \quad (\text{B6})$$

The expression of spherical harmonics can be expressed in terms of Legendre functions as follows:

$$Y_{n,m}(\theta, \phi) = \begin{cases} \sqrt{2} K_n^m \cos(m\phi) P_n^m(\cos \theta) (-1)^m, & m > 0, \\ \sqrt{2} K_n^m \sin(-m\phi) P_n^{-m}(\cos \theta) (-1)^m, & m < 0, \\ K_n^0 P_n^0(\cos \theta), & m = 0. \end{cases} \quad (\text{B7})$$

$$K_n^m = \sqrt{\frac{(2n+1)}{4\pi} \frac{(n-|m|)!}{(n+|m|)!}}. \quad (\text{B8})$$

Switching from spherical to Cartesian coordinates, the formula for spherical harmonics is given by

$$\begin{aligned} r^n Y_{n,m} &= \sqrt{\frac{2n+1}{2\pi}} \sum_{k=0}^{(n-m)/2} \sum_{r=0}^k \sum_{s=0}^{k-r} \sum_{p=0}^m \\ & \quad \times f_{k,r,s,p}^{n,m} x^{p+2r} y^{-p+2s+m} z^{n-2r-2s-m}, \\ f_{k,r,s,p}^{n,m} &= \left[(-1)^k (2n-2k)! \cos\left(\frac{\pi}{2}(m-p)\right) C_m^p \right] \\ & \quad / [2^n r! s! (k-r-s)! (n-k)! (n-2k-m)! m!] \\ & \quad / [\sqrt{(n+m)!/(n-m)!} / m!], \end{aligned} \quad (\text{B9})$$

which is suitable for straight magnetic elements [30].

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