THE RAY-TRACING CODE ZGOUBI

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Abstract

The ray-tracing code ZGOUBI computes charged particle trajectories in magnetic and/or electric fields. It is dedicated to the definition, design, and study of— and tracking in—optical elements, beam lines, spectrometers, and other periodic structures. The code is a genuine compendium of numerical recipes dedicated to the simulation of most types and geometries of magnetic and/or electric fields encountered in beam optics. It can read and process direct output 1D to 3D field maps from the POISSON and TOSCA programs. ZGOUBI also contains a built-in fitting procedure dedicated to the optimization of fields, geometry, acceptance, and numerous numerical means based on Monte Carlo processes.

Ray-tracing is performed by a stepwise resolution of the Lorentz equation of motion,

$$d\vec{p}/dt = q(\vec{e} + \vec{v} \times \vec{b}) ,$$

($\vec{p}$ = momentum, q = charge, $\vec{e}$ = electric field, $\vec{b}$ = magnetic field) by a method of Taylor expansions of the particle position $\vec{R}$ and velocity $\vec{v}$ vectors. The method is described and illustrated by a multiturn tracking simulation in a proton synchrotron. Optionally, ZGOUBI solves in a similar way the Thomas-BMT spin transport equation

$$d\vec{S}/dt = (q/m)\vec{S} \times \vec{\Omega} ,$$

($\vec{S}$ = spin, m = mass, $\Omega = (1 + \gamma G) \vec{b} + G(1 - \gamma) \vec{b}_{\parallel}$, with $\vec{b}_{\parallel} = (1/v^2) (\vec{b} \cdot \vec{v}) \vec{v}$, γ = Lorentz relativistic factor, G = anomalous magnetic moment). This is illustrated by a simulation of spin resonance crossing in a proton synchrotron. If required, the code performs a stepwise calculation of the synchrotron radiation electric field,

$$\vec{E}(\tau) = \left(\frac{q}{4\pi\epsilon_0 c} \right) \vec{n}(t) \times [(\vec{n}(t) - \vec{\beta}(t)) \times d\vec{\beta}/dt] / r(t) [1 - \vec{n}(t) \cdot \vec{\beta}(t)]^3 ,$$

(τ = observer time, $\epsilon_0 = 1/\mu_0 c^2$, $\mu_0 = 4\pi \times 10^{-7}$, c = light velocity, $\vec{n}$ = particle to observer direction, $\vec{\beta} = \vec{v}/c$), and other associated spectral brightness. A calculation of synchrotron radiation interferences illustrates this.

Three typical procedures are also described: the fitting procedure FIT; the DIPOLE procedure that generates a 2D median plane field map; and the MULTIPOLE procedure which simulates the field of a multipole magnet. An application of these to an inverse problem is presented: the optimization of a QD spectrometer is shown, involving the fitting procedure for field and geometry optimizations.

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1 INTRODUCTION

The computer code ZGOUBI calculates trajectories of charged particles in magnetic and/or electric fields. Especially adapted for the definition and adjustment of beam lines and magnetic spectrometers, it allows the study of systems including complex sequences of optical magnetic and/or electric devices. Compared to other codes, it presents several peculiarities:

- a numerical method for integrating the Lorentz equation, based on the Taylor series, which optimizes the computing time and provides high accuracy
- spin tracking
- calculation of synchrotron radiation in arbitrary magnetic fields
- the possibility of using a mesh, which allows ray-tracing from simulated or measured (1D, 2D or 3D) field maps
- Monte Carlo procedures: unlimited number of trajectories, in-flight decay, etc.
- a built-in fitting procedure
- multiturn tracking in periodic structures (including the simulation of synchrotron acceleration and time-varying power supplies).

The initial version of the Code, limited to ray-tracing in magnetic fields, was developed at CEA-Saclay in the early 1970's [1]. Since then many improvements have been implemented and a users' guide has been written and is periodically upgraded [2].

2 NUMERICAL METHODS FOR THE TRACKING OF PARTICLES, SPIN, AND SYNCHROTRON RADIATION

2.1 Integration of the Lorentz Equation

The reference frame of ZGOUBI is presented in Fig. 1. Its origin is in the median plane on a reference curve which coincides with the optical axis of optical elements.

Figure 1: Reference frame and coordinates (Y , T , Z , P) in ZGOUBI.
 OX : in the plane of the reference curve in the direction of motion,
 OY : in the plane of the reference curve, normal to OX ,
 OZ : orthogonal to the reference plane,
 $\vec{W}$: projection of the velocity, $\vec{v}$, in the plane of the reference curve,
 T = angle between $\vec{W}$ and the X axis,
 P = angle between $\vec{W}$ and $\vec{v}$.

The Lorentz equation, which governs the motion of a particle of charge q , mass m , and velocity $\vec{v}$ in electric and magnetic fields $\vec{e}$ and $\vec{b}$, is written:

$$\frac{d(m\vec{v})}{dt} = q(\vec{e} + \vec{v} \times \vec{b}) . \quad (2.1.1)$$

Taking (Ref. [3]),

$$\vec{u} = \frac{\vec{v}}{v} , \quad ds = v dt , \quad \vec{u}' = \frac{d\vec{u}}{ds} , \quad m\vec{v} = mv\vec{u} = q B\rho \vec{u} , \quad (2.1.2)$$

where $B\rho$ is the rigidity of the particle, this equation can be rewritten:

$$(B\rho)'\vec{u} + B\rho \vec{u}' = \frac{\vec{e}}{v} + \vec{u} \times \vec{b} . \quad (2.1.3)$$

From the position $\vec{R}(M_0)$ and unit velocity $\vec{u}(M_0)$ at point M_0 , the position $\vec{R}(M_1)$ and unit velocity $\vec{u}(M_1)$ at point M_1 following a displacement ds (Fig. 2) are given by Taylor expansions

$$\begin{aligned} \vec{R}(M_1) &= \vec{R}(M_0) + \vec{u}(M_0)ds + \vec{u}'(M_0) \frac{ds^2}{2!} + \dots + \vec{u}''''(M_0) \frac{ds^6}{6!} \\ \vec{u}(M_1) &= \vec{u}(M_0) + \vec{u}'(M_0)ds + \vec{u}''(M_0) \frac{ds^2}{2!} + \dots + \vec{u}''''(M_0) \frac{ds^5}{5!} . \end{aligned} \quad (2.1.4)$$

The rigidity at M_1 is obtained in the same way from

$$(B\rho)(M_1) = (B\rho)(M_0) + (B\rho)'(M_0)ds + \dots + (B\rho)''''(M_0) \frac{ds^4}{4!} . \quad (2.1.5)$$

The derivatives $\vec{u}^{(n)} = d^n \vec{u} / ds^n$ and $(B\rho)^{(n)} = d^n (B\rho) / ds^n$ involved in these expressions are calculated as described below.

Figure 2: Position and velocity of a particle in the reference frame.

Successive differentiations of Eq. (2.1.3) give the recursive relations

$$\begin{aligned}
(B\rho)'\vec{u} + B\rho\vec{u}' &= \frac{\vec{e}}{v} + \vec{u} \times \vec{b} \\
(B\rho)''\vec{u} + 2(B\rho)'\vec{u}' + B\rho\vec{u}'' &= \left(\frac{1}{v}\right)'\vec{e} + \left(\frac{1}{v}\right)\vec{e}' + (\vec{u} \times \vec{b})' \\
(B\rho)'''\vec{u} + 3(B\rho)''\vec{u}' + 3(B\rho)'\vec{u}'' + B\rho\vec{u}''' &= \left(\frac{1}{v}\right)''\vec{e} + 2\left(\frac{1}{v}\right)'\vec{e}' + \left(\frac{1}{v}\right)\vec{e}'' + (\vec{u} \times \vec{b})'' \\
(B\rho)''''\vec{u} + 4(B\rho)'''\vec{u}' + 6(B\rho)''\vec{u}'' + 4(B\rho)'\vec{u}''' + B\rho\vec{u}'''' &= \\
&\left(\frac{1}{v}\right)'''\vec{e} + 3\left(\frac{1}{v}\right)''\vec{e}' + 3\left(\frac{1}{v}\right)'\vec{e}'' + \frac{1}{v}\vec{e}''' + (\vec{u} \times \vec{b})''' ,
\end{aligned} \tag{2.1.6}$$

that provide the derivatives $d^n\vec{u}/ds^n$ as needed in the Taylor expansions (2.1.4):

$$\begin{aligned}
\vec{u}' &= \left(\frac{1}{v}\right)\vec{E} + (\vec{u} \times \vec{B}) - \frac{(B\rho)'}{B\rho}\vec{u} \\
\vec{u}'' &= \left(\frac{1}{v}\right)'\vec{E} + \left(\frac{1}{v}\right)\vec{E}'|_{B\rho} + (\vec{u} \times \vec{B})'|_{B\rho} - 2\frac{(B\rho)'}{B\rho}\vec{u}' - \frac{(B\rho)''}{B\rho}\vec{u} \\
\vec{u}''' &= \left(\frac{1}{v}\right)''\vec{E} + 2\left(\frac{1}{v}\right)'\vec{E}'|_{B\rho} + \frac{1}{v}\vec{E}''|_{B\rho} + (\vec{u} \times \vec{B})''|_{B\rho} - 3\frac{(B\rho)'}{B\rho}\vec{u}'' - 3\frac{(B\rho)''}{B\rho}\vec{u}' - \frac{(B\rho)'''}{B\rho}\vec{u} \\
\vec{u}'''' &= \left(\frac{1}{v}\right)'''\vec{E} + 3\left(\frac{1}{v}\right)''\vec{E}'|_{B\rho} + 3\left(\frac{1}{v}\right)'\vec{E}''|_{B\rho} + \left(\frac{1}{v}\right)\vec{E}'''|_{B\rho} \\
&+ (\vec{u} \times \vec{B})'''|_{B\rho} - 4\frac{(B\rho)'}{B\rho}\vec{u}''' - 6\frac{(B\rho)''}{B\rho}\vec{u}'' - 4\frac{(B\rho)'''}{B\rho}\vec{u}' - \frac{(B\rho)''''}{B\rho}\vec{u} ,
\end{aligned} \tag{2.1.7}$$

where $\vec{E} = \vec{e}/B\rho$, $\vec{B} = \vec{b}/B\rho$, while $^{(n)}|_{B\rho}$ denotes differentiation at constant $B\rho$:

$$\vec{E}^{(n)}|_{B\rho} = \frac{1}{B\rho} \frac{d^n\vec{e}}{ds^n} \quad \text{and} \quad (\vec{u} \times \vec{B})^{(n)}|_{B\rho} = \frac{1}{B\rho} (\vec{u} \times \vec{b})^{(n)} . \tag{2.1.8}$$

The following recursive formulae are used to calculate these derivatives $^{(n)}|_{B\rho}$.

On the one hand, a simple differentiation gives

$$\begin{aligned}
(\vec{u} \times \vec{b})' &= \vec{u}' \times \vec{b} + \vec{u} \times \vec{b}' \\
(\vec{u} \times \vec{b})'' &= \vec{u}'' \times \vec{b} + 2\vec{u}' \times \vec{b}' + \vec{u} \times \vec{b}'' \\
(\vec{u} \times \vec{b})''' &= \vec{u}''' \times \vec{b} + 3\vec{u}'' \times \vec{b}' + 3\vec{u}' \times \vec{b}'' + \vec{u} \times \vec{b}''' \\
(\vec{u} \times \vec{b})'''' &= \vec{u}'''' \times \vec{b} + 4\vec{u}''' \times \vec{b}' + 6\vec{u}'' \times \vec{b}'' + 4\vec{u}' \times \vec{b}''' + \vec{u} \times \vec{b}'''' ,
\end{aligned} \tag{2.1.9}$$

where $\vec{b}^{(n)} = d^n\vec{b}/ds^n$.

On the other hand, from

$$d\vec{b} = \frac{\partial\vec{b}}{\partial X}dX + \frac{\partial\vec{b}}{\partial Y}dY + \frac{\partial\vec{b}}{\partial Z}dZ = \sum_{i=1,3} \frac{\partial\vec{b}}{\partial X_i}dX_i ,$$

and by successive differentiation, the derivatives $\vec{b}^{(n)}$ write:

$$\vec{b}' = \sum_i \frac{\partial\vec{b}}{\partial X_i} u_i$$

$$\begin{aligned}
\vec{b}'' &= \sum_{ij} \frac{\partial^2 \vec{b}}{\partial X_i \partial X_j} u_i u_j + \sum_i \frac{\partial \vec{b}}{\partial X_i} u_i' \\
\vec{b}''' &= \sum_{ijk} \frac{\partial^3 \vec{b}}{\partial X_i \partial X_j \partial X_k} u_i u_j u_k + 3 \sum_{ij} \frac{\partial^2 \vec{b}}{\partial X_i \partial X_j} u_i' u_j + \sum_i \frac{\partial \vec{b}}{\partial X_i} u_i'' \\
\vec{b}^{(4)} &= \sum_{ijkl} \frac{\partial^4 \vec{b}}{\partial X_i \partial X_j \partial X_k \partial X_l} u_i u_j u_k u_l + 6 \sum_{ijk} \frac{\partial^3 \vec{b}}{\partial X_i \partial X_j \partial X_k} u_i' u_j u_k \\
&\quad + 4 \sum_{ij} \frac{\partial^2 \vec{b}}{\partial X_i \partial X_j} u_i'' u_j + 3 \sum_{ij} \frac{\partial^2 \vec{b}}{\partial X_i \partial X_j} u_i' u_j' + \sum_i \frac{\partial \vec{b}}{\partial X_i} u_i'''
\end{aligned} \tag{2.1.10}$$

Similarly, the derivatives of the electric field are obtained from the total derivative

$$d\vec{e} = \frac{\partial \vec{e}}{\partial X} dX + \frac{\partial \vec{e}}{\partial Y} dY + \frac{\partial \vec{e}}{\partial Z} dZ, \tag{2.1.11}$$

by successive differentiations that give

$$\begin{aligned}
\vec{e}' &= \sum_i \frac{\partial \vec{e}}{\partial X_i} u_i \\
\vec{e}'' &= \sum_{ij} \frac{\partial^2 \vec{e}}{\partial X_i \partial X_j} u_i u_j + \sum_i \frac{\partial \vec{e}}{\partial X_i} u_i' \\
\vec{e}''' &= \sum_{ijk} \frac{\partial^3 \vec{e}}{\partial X_i \partial X_j \partial X_k} u_i u_j u_k + 3 \sum_{ij} \frac{\partial^2 \vec{e}}{\partial X_i \partial X_j} u_i' u_j + \sum_i \frac{\partial \vec{e}}{\partial X_i} u_i''
\end{aligned} \tag{2.1.12}$$

Now, the Eq. (2.1.7), as well as the calculation of the rigidity, following Eq. (2.1.5), involve the derivatives $(B\rho)^{(n)} = d^n(B\rho)/ds^n$, which are obtained in the following way. Considering that

$$\frac{dp^2}{dt} = \frac{d\vec{p}^2}{dt}, \quad \text{i.e.,} \quad \frac{dp}{dt} p = \frac{d\vec{p}}{dt} \vec{p}, \tag{2.1.13}$$

with $d\vec{p}/dt = q(\vec{e} + \vec{v} \times \vec{b})$ (Eq. 2.1.1), we obtain

$$\frac{dp}{dt} p = q(\vec{e} + \vec{v} \times \vec{b}) \cdot \vec{p} = q\vec{e} \cdot \vec{p}, \tag{2.1.14}$$

since $(\vec{v} \times \vec{b}) \cdot \vec{p} = 0$. Normalizing as previously with $\vec{p} = p\vec{u} = qB\rho\vec{u}$ and $ds = vdt$, and by successive differentiations, Eq. (2.1.14) leads to the $(B\rho)^{(n)}$

$$\begin{aligned}
(B\rho)' &= \frac{1}{v}(\vec{e} \cdot \vec{u}) \\
(B\rho)'' &= \left(\frac{1}{v}\right)'(\vec{e} \cdot \vec{u}) + \frac{1}{v}(\vec{e} \cdot \vec{u})' \\
(B\rho)''' &= \left(\frac{1}{v}\right)''(\vec{e} \cdot \vec{u}) + 2\left(\frac{1}{v}\right)'(\vec{e} \cdot \vec{u})' + \frac{1}{v}(\vec{e} \cdot \vec{u})'' \\
(B\rho)^{(4)} &= \left(\frac{1}{v}\right)'''(\vec{e} \cdot \vec{u}) + 3\left(\frac{1}{v}\right)''(\vec{e} \cdot \vec{u})' + 3\left(\frac{1}{v}\right)'(\vec{e} \cdot \vec{u})'' + \frac{1}{v}(\vec{e} \cdot \vec{u})'''
\end{aligned} \tag{2.1.15}$$

Note that the $(\vec{e} \cdot \vec{u})^{(n)} = d^n(\vec{e} \cdot \vec{u})/ds^n$ can be related to the derivatives of the kinetic energy W by

$$dW = \frac{d\vec{p}}{dt} \cdot \vec{v} dt = q\vec{e} \cdot \vec{v} dt, \tag{2.1.16}$$

which, by noting $ds = vdt$ and $\vec{u} = \vec{v}/v$, gives $d^{n+1}W/ds^{n+1} = q d^n(\vec{e} \cdot \vec{u})/ds^n$.

Finally, the derivatives $(1/v)^{(n)} = d^n(1/v)/ds^n$ involved in Eqs. (2.2.10) and (2.2.15) are obtained from $p = v/c W + mc^2/c$, by successive differentiations, that give the recursive relations

$$\begin{aligned} \left(\frac{1}{v}\right) &= \frac{1}{c^2} \frac{W + mc^2}{qB\rho} \\ \left(\frac{1}{v}\right)' &= \frac{1}{c^2} \frac{(\vec{e} \cdot \vec{u})}{B\rho} - \frac{1}{v} \frac{(B\rho)'}{B\rho} \\ \left(\frac{1}{v}\right)'' &= \frac{1}{c^2} \frac{(\vec{e} \cdot \vec{u})'}{B\rho} - 2\left(\frac{1}{v}\right)' \frac{(B\rho)'}{B\rho} - \frac{1}{v} \frac{(B\rho)''}{B\rho} \\ \left(\frac{1}{v}\right)''' &= \frac{1}{c^2} \frac{(\vec{e} \cdot \vec{u})''}{B\rho} - 3\left(\frac{1}{v}\right)'' \frac{(B\rho)'}{B\rho} - 3\left(\frac{1}{v}\right)' \frac{(B\rho)''}{B\rho} - \frac{1}{v} \frac{(B\rho)'''}{B\rho} . \end{aligned} \quad (2.1.17)$$

Remark: Most of the equations above simplify drastically when either $\vec{e}$ or $\vec{b}$ is zero. Therefore, for the sake of computing speed, three distinct procedures have been implemented in the code. The relevant one is called for the step by step integration, depending on whether e or b is zero, or both e and b are non-zero.

An example: Multiturn tracking in a proton synchrotron

Although not specific of the use of the ray-tracing code ZGOUBI, the stringency of multiturn tracking makes it a very good test of the efficiency of the integration method and of such characteristics as symplecticity.

Figure 3: Optical functions of the SATURNE proton synchrotron, as obtained from a preliminary design with a regular matrix code (including a gradient perturbation of 1% in one of the lattice quadrupoles). The Twiss functions so-obtained are, at $s = 0$, $\beta_y = 15.18$ m, $\gamma_y = 0.581$ m⁻¹ (horizontal) and $\beta_z = 2.063$ m, $\gamma_z = 0.572$ m⁻¹ (vertical). The corresponding theoretical (perturbed) tunes are $\nu_y/\nu_z = 3.6375/3.6089$.

The model of the ring used here for the tracking is schemed in terms of its optical functions in Fig. 3 (namely, the SATURNE 3 GeV synchrotron [4]: 4-fold periodicity,

magnetic radius = 6.3381 m, geometrical radius = 16.8 m, perimeter = 105.6 m. Note that, for the purpose of the next section, the machine tuning accounts for a gradient perturbation of 1% in one of the lattice quadrupoles). The tunes are $\nu_y/\nu_z = 3.6375/3.6089$. An integration step size of $ds = 1.5$ cm is taken in all the magnets (sixteen 2.47 m long dipoles and twenty-four 0.48 m long quadrupoles). This results in about 3400 integration steps per machine turn. The investigations performed on the efficiency of the numerical method by means of this tracking trial are summarized and commented in Fig. 4 and its caption.

Figure 4: Tracking of a particle over 3000 turns. These calculations show how precisely the first-order parameters of motion are reproduced by the multiturn ray-tracing. (a) Horizontal phase-space. The particle starts nearby the horizontal closed orbit and with $z_0 = z'_0 = 0$. Due to the numerical imprecision the 3000 phase-space points undergo spreading, but with negligible extent ($\varepsilon_y/\pi \simeq 0$). (b) Vertical phase-space. The particle starts with $z_0 = 4.58 \times 10^{-3}$ m, $z'_0 = 0$. A least-square fit by the ellipse $\gamma_z z^2 + 2\alpha_z z z' + \beta_z z'^2 = \varepsilon_z/\pi$ gives $\beta_z = 2.05$ m, $\gamma_z = 0.582$ m $^{-1}$, $\varepsilon_z/\pi = 12.2 \times 10^{-6}$ m·rad in accordance with the preliminary matrix calculations (Fig. 3). (c) Tune numbers obtained by Fourier analysis of the phase-space ellipses for $\varepsilon_y/\pi = \varepsilon_z/\pi \simeq 12 \times 10^{-6}$ m·rad : $\nu_y = 3.6375$, $\nu_z = 3.6088$; again these values are correct. (d) Longitudinal phase-space. The particles are accelerated at a rate of 1405 eV/turn ($\dot{B} = 2.1$ T/s) with a momentum dispersion of 5×10^{-4} (1), 10^{-3} (2), 1.65×10^{-3} (3) (the motion is then outside the separatrix); note that analytical calculations give accordingly a momentum acceptance of 1.65×10^{-3} . These four figures show the efficiency of the numerical ray-tracing.

2.2 Spin tracking [5]

The motion of the spin $\vec{S}$ of a charged particle is governed by the Thomas-BMT first-order differential equation [6]:

$$\frac{d\vec{S}}{dt} = \frac{q}{m} \vec{S} \times \vec{\Omega} , \quad (2.2.1)$$

where

$$\vec{\Omega} = (1 + \gamma G)\vec{b} + G(1 - \gamma)\vec{b}_{\parallel} . \quad (2.2.2)$$

q , m , γ and G are respectively the charge, mass, Lorentz relativistic factor, and anomalous magnetic moment of the particle. $\vec{b}_{\parallel}$ is the component of $\vec{b}$ which is parallel to the velocity $\vec{v}$ of the particle.

These equations are normalized by introducing the same notation as previously. Let $b = \|\vec{b}\|$ and $v = \|\vec{v}\|$; $ds = vdt$ is the differential path, $mv/q = B\rho$ is the rigidity of the particle; $\vec{S}' = d\vec{S}/ds = 1/v d\vec{S}/dt$ is the derivative of the spin with respect to the path.

Introducing also $\vec{B} = \vec{b}/B\rho$ and $\vec{B}_{\parallel} = \vec{b}_{\parallel}/B\rho$, and

$$\vec{\omega} = \frac{\vec{\Omega}}{B\rho} = (1 + \gamma G)\vec{B} + G(1 - \gamma)\vec{B}_{\parallel} , \quad (2.2.3)$$

Eq. (2.2.2) can be rewritten in a normalized way

$$\vec{S}' = \vec{S} \times \vec{\omega} . \quad (2.2.4)$$

This equation is then solved in the same way as we did for the Lorentz equation. From the values of the magnetic factor $\vec{\omega}(M_0)$ and the spin $\vec{S}(M_0)$ of the particle at position M_0 of its trajectory, the spin $\vec{S}(M_1)$ at position M_1 , following a displacement ds (Fig. 2), is given by the Taylor expansion

$$\vec{S}(M_1) = \vec{S}(M_0) + \frac{d\vec{S}}{ds}(M_0)ds + \frac{d^2\vec{S}}{ds^2}(M_0)\frac{ds^2}{2} + \frac{d^3\vec{S}}{ds^3}(M_0)\frac{ds^3}{3!} + \frac{d^4\vec{S}}{ds^4}(M_0)\frac{ds^4}{4!} . \quad (2.2.5)$$

The derivatives $\vec{S}^{(n)} = d^n\vec{S}/ds^n$ of $\vec{S}$ at M_0 are obtained by differentiating Eq. (2.2.4):

$$\begin{aligned} \vec{S}' &= \vec{S} \times \vec{\omega} \\ \vec{S}'' &= \vec{S}' \times \vec{\omega} + \vec{S} \times \vec{\omega}' \\ \vec{S}''' &= \vec{S}'' \times \vec{\omega} + 2\vec{S}' \times \vec{\omega}' + \vec{S} \times \vec{\omega}'' \\ \vec{S}^{(4)} &= \vec{S}''' \times \vec{\omega} + 3\vec{S}'' \times \vec{\omega}' + 3\vec{S}' \times \vec{\omega}'' + \vec{S} \times \vec{\omega}''' , \end{aligned} \quad (2.2.6)$$

where the derivatives $\vec{\omega}^{(n)}$ are obtained from Eq. (2.2.3).

The last point consists in getting $\vec{B}_{\parallel}$ and its derivatives. This can be done in the following way. Let $\vec{u} = \vec{v}/v$ be the normalized velocity of the particle, then,

$$\begin{aligned} \vec{B}_{\parallel} &= (\vec{B} \cdot \vec{u})\vec{u} \\ \vec{B}'_{\parallel} &= (\vec{B}' \cdot \vec{u} + \vec{B} \cdot \vec{u}')\vec{u} + (\vec{B} \cdot \vec{u})\vec{u}' \\ \vec{B}''_{\parallel} &= (\vec{B}'' \cdot \vec{u} + 2\vec{B}' \cdot \vec{u}' + \vec{B} \cdot \vec{u}'')\vec{u} + 2(\vec{B}' \cdot \vec{u} + \vec{B} \cdot \vec{u}')\vec{u}' + (\vec{B} \cdot \vec{u})\vec{u}'' \\ &\text{etc...} \end{aligned} \quad (2.2.7)$$

The quantities $\vec{u}$, $\vec{B}$ and their n-th derivatives as involved in these equations are picked up from Eqs. (2.1.9) and (2.1.10).

An example: spin resonance crossing

Again, though not very specific of the use of ZGOUBI, multiturn spin tracking is a stringent test of the accuracy and symplecticity of the integration method, as applied to the Thomas-BMT first-order differential equation. Nonetheless, the simulations can be straightforwardly compared with analytical results such as the Froissard-Stora formula [7]. Again, we consider the SATURNE synchrotron (Figs. 3, 4). Figure 5 shows the crossing of the quadrupole resonance $\gamma G = 7 - \nu_z$ [8].

Figure 5: Crossing of $\gamma G = 7 - \nu_z$ at an acceleration rate of $\text{dB}/\text{dt} = 2.1 \text{ T/s}$, on the invariants $\varepsilon_y/\pi = 0$ and (a) $\varepsilon_z/\pi = 12.2 \times 10^{-6} \text{ m-rad}$ or (b) $\varepsilon_z/\pi = 1.22 \times 10^{-6} \text{ m-rad}$. From these simulations, the strength of the resonance can be calculated to be (a) $|\varepsilon| = 3.29 \times 10^{-4}$, or (b) $|\varepsilon| = 1.04 \times 10^{-4}$, proportional to $\sqrt{\varepsilon_z}$ in agreement with the theory. The asymptotic polarization is also in excellent agreement with the Froissard-Stora formula for an isolated resonance [7] $S_z(t = \infty)/S_z(t = -\infty) = 2 \exp(-\pi m |\varepsilon|^2/2 G R \text{ dB}/\text{dt})$ namely, (a) $S_z(t = \infty)/S_z(t = -\infty) = 0.44$ or (b) $S_z(t = \infty)/S_z(t = -\infty) = 0.92$. The case (c) cannot be attained with analytical means: it shows the behaviour of $S_z(t)$ for an off-momentum particle subject to synchrotron motion with a maximum amplitude $\delta p/p = 10^{-3}$ [Fig. 4(d)].

2.3 Calculation of the synchrotron radiation [9]

The ray-tracing procedures as described in Section 2.1 provide the ingredients necessary for the determination of the electric field radiated by the particle subject to acceleration, as shown in Fig. 6.

Figure 6: A scheme of the reference frame in ZGOUBI together with the vectors entering in the definition of the electric field radiated by the accelerated particle:

(x,y): horizontal plane; z: vertical axis.

$\vec{R}(t)$ = particle position in the fixed frame (O, x, y, z);

$\vec{x}$ (time-independent) = position of the observer in the (O, x, y, z) frame;

$\vec{r}(t) = \vec{x} - \vec{R}(t)$ = position of the particle with respect to the observer;

$\vec{n}(t)$ = (normalized) direction of observation = $\vec{r}(t)/|\vec{r}(t)|$;

$\vec{\beta}$ = normalized velocity vector of the particle $\vec{v}/c = (1/c)d\vec{R}/dt$.

2.3.1 Calculation of the electric field $\mathcal{E}(\vec{n}, \tau)$

The expression for $\mathcal{E}(\vec{n}, \tau)$ as seen by the observer in the long distance approximation is [10]

$$\mathcal{E}(\vec{n}, \tau) = \frac{q}{4\pi\epsilon_0 c} \frac{\vec{n}(t) \times [(\vec{n}(t) - \vec{\beta}(t)) \times d\vec{\beta}/dt]}{r(t)(1 - \vec{n}(t) \cdot \vec{\beta}(t))^3}, \quad (2.3.1)$$

where t is the time in which the particle motion is described and τ is the observer time. Namely, when at position $\vec{r}(t)$ with respect to the observer [or as well at position $\vec{R}(t) = \vec{x} - \vec{r}(t)$ in the (O, x, y, z) frame] the particle emits a signal which reaches the observer at time τ , such that $\tau = t + r(t)/c$ where $r(t)/c$ is the delay necessary for the signal to travel from the emission point to the observer, which also leads by differentiation to the well-known differential relation

$$d\tau/dt = 1 - \vec{n}(t) \cdot \vec{\beta}(t).$$

The vectors $\vec{R}(t)$ and $\vec{\beta}(t)$ that describe the motion are obtained from the ray-tracing (Eqs. 2.1.4). The acceleration is calculated from (Eq. 2.1.1)

$$d\vec{\beta}/dt = (q/m) \vec{\beta}(t) \times \vec{b}(t).$$

Then, given the observer position $\vec{x}$ in the fixed frame, it is possible to calculate

$$\vec{r}(t) = \vec{x} - \vec{R}(t) \quad \text{and} \quad \vec{n}(t) = \vec{r}(t)/|\vec{r}(t)|.$$

The calculation of $\vec{n} - \vec{\beta}$ and $1 - \vec{n} \cdot \vec{\beta}$ related to computer precision.

In principle, owing to computer precision the crude computation of $\vec{n} - \vec{\beta}$ and $1 - \vec{n} \cdot \vec{\beta}$ will, most of the time (i.e. over large $\vec{n}$ or t ranges), lead to

$$\vec{n} - \vec{\beta} = 0 \quad \text{and} \quad 1 - \vec{n} \cdot \vec{\beta} = 0,$$

since the preferred direction of observation is generally almost parallel to $\vec{\beta}$ (exactly parallel in the sense of computer precision), while $\beta \approx 1$ as soon as particle energies of a few hundred times the rest mass are concerned.

It is therefore necessary to express $\vec{n} - \vec{\beta}$ and $1 - \vec{n} \cdot \vec{\beta}$ in an adequate software form for performing the computation.

The expression for $\vec{n}$ is

$$\begin{aligned} \vec{n} &= (\cos \Psi \cos \phi, \cos \Psi \sin \phi, \sin \Psi) \\ &= [1 - 2(\sin^2 \phi/2 + \sin^2 \Psi/2) + 4 \sin^2 \phi/2 \sin^2 \Psi/2, \sin \phi(1 - 2 \sin^2 \Psi/2), \sin \Psi] , \end{aligned} \quad (2.3.2)$$

where ϕ and Ψ are the observation angles, given by

$$\phi = \text{Atg}\left(\frac{r_y}{r_x}\right) \quad \text{and} \quad \Psi = \text{Atg}\left(\frac{r_z}{\sqrt{r_x^2 + r_y^2}}\right) ,$$

with $\vec{r} = (r_x, r_y, r_z)$, while $\vec{\beta}$ can be written under the form

$$\begin{aligned} \vec{\beta} &= (\beta_x, \beta_y, \beta_z) = [\sqrt{(\beta^2 - \beta_y^2 - \beta_z^2)}, \beta_y, \beta_z] , \\ &= [\sqrt{(1 - 1/\gamma^2 - \beta_y^2 - \beta_z^2)}, \beta_y, \beta_z] = (1 - a/2 + a^2/8 - a^3/16 + \dots, \beta_y, \beta_z) , \end{aligned} \quad (2.3.3)$$

where $a = 1/\gamma^2 + \beta_y^2 + \beta_z^2$. We then note

$$\vec{n} = (1 - \varepsilon_x, n_y, n_z) \quad \text{and} \quad \vec{\beta} = (1 - \xi_x, \beta_y, \beta_z) ,$$

with

$$\varepsilon_x = 2(\sin^2 \phi/2 + \sin^2 \Psi/2) - 4 \sin^2 \phi/2 \sin^2 \Psi/2 ,$$

and

$$\xi_x = a/2 - a^2/8 + a^3/16 + \dots$$

All this provides, on the one hand,

$$\vec{n} - \vec{\beta} = (-\varepsilon_x + \xi_x, n_y - \beta_y, n_z - \beta_z) , \quad (2.3.4)$$

whose components are combinations of terms of the same order of magnitude (ε_x and $\xi_x \sim 1/\gamma^2$ while n_y, β_y, n_z and $\beta_z \sim 1/\gamma$) and, on the other hand,

$$1 - \vec{n} \cdot \vec{\beta} = \varepsilon_x + \xi_x - n_y \beta_y - n_z \beta_z - \varepsilon_x \xi_x , \quad (2.3.5)$$

that combines terms of the same order of magnitude ($\varepsilon_x, \xi_x, n_y \beta_y$ and $n_z \beta_z \sim 1/\gamma^2$), plus $\varepsilon_x \beta_x \sim 1/\gamma^4$.

From a practical (programming) point of view, the precision of these expressions is directly related to the order at which the series

$$\xi_x = a/2 - a^2/8 + a^3/16 + \dots \quad (a = 1/\gamma^2 + \beta_y^2 + \beta_z^2)$$

is expanded (the convergence is in principle fast since $a \sim 1/\gamma^2 \ll 1$).

Finally, the electric field is decomposed into the two components $\vec{\mathcal{E}}_\sigma$ (parallel to the bend plane and normal to $\vec{n}$) and $\vec{\mathcal{E}}_\pi$ (normal to $\vec{\mathcal{E}}_\sigma$ and $\vec{n}$).

Calculation of the Fourier transform of the electric field

The Fourier transforms

$$FT_\omega[\mathcal{E}(\tau)] = \int \mathcal{E}(\tau) e^{-i\omega\tau} d\tau ,$$

of the σ and π electric field components provide the spectral angular brightness $\partial^3 P / \partial \phi \partial \Psi \partial \omega$. They are calculated in a regular way, without using the FFT technics, namely from

$$FT_\omega[\mathcal{E}(\tau)] \approx \sum \mathcal{E}(\tau_n) e^{-i\omega\tau_n} \Delta\tau_n , \quad (2.3.6)$$

for two reasons. On the one hand, the number of integration steps ds that define the trajectory (Eqs. 2.1.4), is fully arbitrary and therefore in general not of order 2^n . On the other hand, the integration step defines a constant time differential element $dt = ds/\beta c$ which results in the observer differential time element $d\tau$, which is also the differential element of the Fourier transform, being non-constant, since both are related by

$$d\tau = dt[1 - \vec{n}(t) \cdot \vec{\beta}(t)] .$$

The key point is that $d\tau$ can reach drastically small values in the region of the central peak of the electric impulse (where $1 - \vec{n}(t) \cdot \vec{\beta}(t) \rightarrow 1/2\gamma^2$), while the total integrated time $\tau = \sum \Delta\tau_n$ may be several orders of magnitude larger. Namely, the total duration of the electric field impulse as seen by the observer corresponds to the time delay that separates photons emitted at the entrance of the magnet from photons emitted at the exit, but the significant part of it (in terms of energy density) which can be represented by the width of the peak of radiation [e.g., at $\mathcal{E}_\sigma(\tau) = 0$], is a very small fraction of that delay, namely [11]

$$2\tau_c = \frac{2(1 + \gamma^2\psi^2)^{3/2}}{3\gamma^3} \frac{2\rho}{c} . \quad (2.3.7)$$

For instance, at $\gamma \approx 8.8 \times 10^4$ (45 GeV electrons), with a magnet of bending radius $\rho = 876.7$ m and length 0.526 m, the total duration of the electric field impulse (from the entrance to the exit of the magnet) is of the order of 2.6×10^{-17} s, while $\tau_c \approx 2.85 \times 10^{-21}$ s, both for an observation angle $\Psi = 0$.

The consequence is that, once again in relation with computer precision, the differential element $\Delta\tau_n$ involved in the computation of

$$FT_\omega[\mathcal{E}(\tau)] \approx \sum \mathcal{E}(\tau_n) e^{-i\omega\tau_n} \Delta\tau_n$$

cannot be derived from such relation as $\Delta\tau_n = \tau_n - \tau_{n-1}$, but instead must be stored as such beforehand.

An example: Synchrotron radiation interferences

Figure 7 schemes a set-up involving two small dipole magnets. The two electric field impulses emitted by a single particle that crosses successively the two magnets are observed at a large distance in the (arbitrary) direction $\gamma\Psi = 10$ off the bend plane; they give a typical interference-like frequency spectrum, whose modulation frequency depends on the distance between the magnets [9]. The results of the ray-tracing simulations and their high degree of precision are shown in Fig. 8 and its caption.

Figure 7: A particle crosses two neighbouring small dipoles W_1 and W_2 , distance d , in which it undergoes a deflection α , which results in the emission of a double electromagnetic radiation impulse. The time delay between the two successive impulses, as observed at a large distance in the direction $\gamma\Psi$ off the bend plane, is $T = d (1 + \gamma^2\Psi^2 + \alpha^2\gamma^2/8)/2\gamma^2c$.

Figure 8: (a) The electric field component E_σ of the double impulse emitted successively in W_1 and W_2 , as observed at a large distance in the direction $\gamma\Psi$ off the bend plane. With the present conditions: 45 GeV electrons ($\gamma = 88 \times 10^3$), $\alpha = 0.6 \times 10^{-3}$ rad, $d = 75.7 \times 10^{-2}$ m and $\gamma\Psi = 10$, the time delay between the two successive impulses, from the expression given in Fig. 7, is $T = 7.326 \times 10^{-17}$ s, which with a very high accuracy is what the ray-tracing provides. (b) The radiation spectrum, obtained by Fourier transforming of the previous electric field double impulse as obtained from the ray-tracing, shows a characteristic interference-like pattern in perfect agreement with the theory: a modulation coefficient $\sin^2(\omega T/2)$ of frequency $1/T = 56.45$ eV [9], and an envelope which identifies with the classical synchrotron radiation spectrum of the dipole magnet, i.e., of the $K_{2/3}^2$ form [10] (apart from the region $\omega \simeq \sigma$, in the present case of small dipoles – see Ref. [9] for more details).

3 THREE TYPICAL PROCEDURES [2]

3.1 FIT: the fitting procedure

The fitting procedure FIT allows the automatic adjustment of up to 20 variables, for up to 20 constraints. It has been carried out with existing routines used in the matrix transport code BETA [12]. Any physical parameter of any element may be varied. Available constraints are: any of the 6×6 coefficients of the equivalent first-order transfer matrix $[R_{ij}]$ (as calculated from a set of 11 paraxial trajectories), and its horizontal ($R_{11}R_{22} - R_{12}R_{21}$) and vertical ($R_{33}R_{44} - R_{34}R_{43}$) determinants; any of the $6 \times 6 \times 6$ coefficients of the equivalent second-order array $[T_{ijk}]$ (calculated from a set of 61 paraxial trajectories); any of the 2×4 coefficients of the beam matrix as defined by

$$[\sigma_{ij}] = \begin{pmatrix} \sigma_{11} & \sigma_{12} & & & & \\ \sigma_{21} & \sigma_{22} & & & & \\ & & \sigma_{33} & \sigma_{34} & & \\ & & \sigma_{43} & \sigma_{44} & & \end{pmatrix},$$

and any trajectory coordinate Y, T, Z, P, X (Fig. 1) and $\delta p/p$ (momentum deviation).

Prior to fitting, the elements are numbered by the code following their sequence in the ZGOUBI input data file. The sequential number of any element just identifies its position in the data list.

In the elements, the numbering of the physical parameters more or less follows their sequence. This numbering of both the optical elements and their parameters allows the user to define the variables of FIT.

The following two examples show the numbering in the case of the DIPOLE and MULTIPOLE procedures, which will be addressed in section 4 (refer to it and to Ref. [2] for more details on the meaning of the numbered parameters).

Input data	Numbering for FIT
DIPOLE	
NFACE, IC, IL	1, 2, 3
IAMAX, IRMAX	4, 5
B ₀ , N, B, G	6, 7, 8, 9
AT, ACENT, RM, RMIN, RMAX	10, 11, 12, 13, 14
λ, ξ	15, 16
NC, C ₀ , C ₁ , C ₂ , C ₃ , C ₄ , C ₅ shift	17, 18, 19, 20, 21, 22, 23, 24
$\omega, \theta, R_1, U_1, U_2, R_2$	25, 26, 27, 28, 29, 30
etc...	etc...

Input data	Numbering for FIT
MULTIPOL	
IL	1
XL, R ₀ , B ₁ , B ₂ , B ₃ , B ₄ , B ₅ , B ₆	10, 11, 12, 13, 14, 15, 16, 17
X _E , λ_E , E ₂ , E ₃ , E ₄ , E ₅ , E ₆	20, 21, 22, 23, 24, 25, 26
NCE, C ₀ , C ₁ , C ₂ , C ₃ , C ₄ , C ₅	30, 31, 32, 33, 34, 35, 36
X _S , λ_S , S ₂ , S ₃ , S ₄ , S ₅ , S ₆	40, 41, 42, 43, 44, 45, 46
NCS, C ₀ , C ₁ , C ₂ , C ₃ , C ₄ , C ₅	50, 51, 52, 53, 54, 55, 56
R ₁ , R ₂ , R ₃ , R ₄ , R ₅ , R ₆	60, 61, 62, 63, 64, 65
XPAS	70
KPOS, XCE, YCE, ALE	80, 81, 82, 83

It is also possible to couple a variable parameter to any other parameter in the structure. Depending on the options, the coupled parameter will be given the same value as the variable parameter (so that for instance, they stay equal) or a variation opposite to it, so that the sum of the two parameters stays constant (for example, an optical element can be shifted while preserving the length of the structure, by coupling together its upstream and downstream drift spaces).

The fitting procedure itself is a direct sequential minimization of the quadratic sum of all errors (i.e. differences between the desired and actual values of the NC constraints), each normalized by a specified weight W [12].

The step sizes for the variation of the physical parameters depend on their initial values, and cannot be accessed by the user. At each iteration, the optimum value of the step size, as well as the optimum direction of variation, is determined for each of the variables. Then follows an iterative global variation of all variables, until the minimization fails, which results in a next iteration on the optimization of the step sizes.

A version of ZGOUBI that uses the Fletcher–Reeves alternated gradient algorithm is available. However, this method was not maintained because it usually gives a slower convergence than the one above, once in the close neighbourhood of the solution [13].

3.2 DIPOLE: Generation of a dipole magnet

The procedure DIPOLE provides an automatic generation of a dipole 2D median plane field map in polar coordinates. The extent of the map is defined by the following parameters, as shown in Figs. 9(a) and 9(b).

AT	: total angular aperture
RM	: mean radius used for the positioning of field boundaries
RMIN, RMAX	: minimum and maximum radii boundaries.

The 2 (or 3, upon option) effective field boundaries (EFB) inside the map are defined from geometric boundaries, the shape and position of which are determined by the following parameters.

ACENT	: arbitrary angle, used for the positioning of field
ω	: azimuth of a boundary with respect to ACENT
θ	: angle of a boundary with respect to its azimuth (wedge angle)
R_1, R_2	: radius of curvature of a boundary
U_1, U_2	: extent of the linear part of a boundary.

At any node of the map mesh, the value of the Z component of the field is calculated as

$$B_z = \mathcal{F} * B_0 * \left[1 + N * \left(\frac{R - RM}{RM} \right) + B * \left(\frac{R - RM}{RM} \right)^2 + G * \left(\frac{R - RM}{RM} \right)^3 \right], \quad (3.2.1)$$

where, N , B and G are, respectively, the first-, second- and third-order field indices, and $\mathcal{F}$ is the fringe field coefficient, while the x and y components of the field are assumed to be zero in the mesh plane.

The fringe field coefficient.

With each EFB a realistic extent of the fringe field, λ (normally equal to the gap size), is associated and a fringe field coefficient F is calculated. In the following λ stands for either λ_E (Entrance), λ_S (Exit) or λ_L (Lateral EFB).

Figure 9: (a) Parameters used to define the field map and geometric boundaries. (b) Parameters used to define the field map and fringe fields.

F is an exponential type fringe given by (Fig. 10)

$$F = \frac{1}{1 + \exp P(s)} \quad , \quad (3.2.2)$$

where s is the distance to the boundary, and

$$P(s) = C_0 + C_1 \left(\frac{s}{\lambda} \right) + C_2 \left(\frac{s}{\lambda} \right)^2 + C_3 \left(\frac{s}{\lambda} \right)^3 + C_4 \left(\frac{s}{\lambda} \right)^4 + C_5 \left(\frac{s}{\lambda} \right)^5.$$

Figure 10: Exponential fringe field.

Let F_E (respectively F_S , F_L) be the fringe field coefficient attached to the entrance (respectively exit, lateral) field boundary. At any node of the map mesh, the resulting value of the fringe field coefficient (Eq. 3.2.1) is

$$\mathcal{F} = F_E * F_S * F_L , \quad (3.2.3)$$

($F_L = 1$ if no lateral face is requested).

The Mesh of the Field Map

The magnetic field is calculated at the nodes of a mesh with polar coordinates, in the median plane. The radial step of the mesh is given by

$$\delta R = \frac{RMAX - RMIN}{IRMAX - 1} ,$$

and the angular step by

$$\delta\theta = \frac{AT}{IAMAX - 1} ,$$

where, IRMAX and IAMAX are the total number of nodes in the radial and angular directions.

Finally, once the initial map is calculated, it is also possible to perturbate it, so as to simulate various types of field defects or shims.

The field interpolation

ZGOUBI provides three types of polynomial interpolation from the mesh (upon option); namely, a second-order interpolation, with either a 9- or a 25-point grid, or a fourth-order interpolation with a 25-point grid.

Let B_{ij} be the value of $B_Z(X, Y, 0)$ at the nodes of the mesh which defines the 2D field map in the (X, Y) plane, while $B_X(X, Y, 0)$ and $B_Y(X, Y, 0)$ are assumed to be zero (Fig. 11).

Figure 11: Mesh in the (X, Y) plane in polar coordinates. The current interpolation grid is centered on the node which is closest to the actual position of the particle.

The interpolation grid is centered on the node which is closest to the projection in the (X, Y) plane of the actual point of the trajectory.

The interpolation polynomial is

$$B_Z(X, Y, 0) = A_{00} + A_{10}X + A_{01}Y + A_{20}X^2 + A_{11}XY + A_{02}Y^2, \quad (3.2.4)$$

in second order, or

$$\begin{aligned} B_Z(X, Y, 0) = & A_{00} + A_{10}X + A_{01}Y + A_{20}X^2 + A_{11}XY + A_{02}Y^2 \\ & + A_{30}X^3 + A_{21}X^2Y + A_{12}XY^2 + A_{03}Y^3 \\ & + A_{40}X^4 + A_{31}X^3Y + A_{22}X^2Y^2 + A_{13}XY^3 + A_{04}Y^4, \end{aligned} \quad (3.2.5)$$

in fourth order. The coefficients A_{ij} are calculated from explicit expressions of the solutions of the normal equations that minimize, with respect to A_{ij} , the quadratic sum

$$\sum_{ij} (B_Z(X, Y, 0) - B_{ij})^2.$$

The A_{ij} may then be identified with the derivatives of $B_Z(X, Y, 0)$ at the central node of the grid:

$$A_{ij} = \frac{1}{i!j!} \frac{\partial^{i+j} B_Z}{\partial X^i \partial Y^j} (0, 0, 0). \quad (3.2.6)$$

The derivatives of $B_Z(X, Y, 0)$ with respect to X and Y , at the actual point $(X, Y, 0)$ are obtained by differentiation of the interpolation polynomial, which gives [e.g. from (3.2.4) in the case of second-order interpolation]

$$\frac{\partial B_Z}{\partial X}(X, Y, 0) = A_{10} + 2A_{20}X + A_{11}Y$$

$$\frac{\partial B_Z}{\partial Y}(X, Y, 0) = A_{01} + A_{11}X + 2A_{02}Y \text{ etc...}$$

This allows stepping to the Z-extrapolation for the calculation of $\vec{B}(X, Y, Z)$ and its derivatives as described further below.

Change of frame from the polar map system to the ZGOUBI cartesian frame.

It is necessary to change from polar to cartesian coordinates since the ray-tracing is performed in cartesian coordinates. This is done as follows.

In second-order calculations the correspondence is [here B stands for $B_Z(X, Y, 0)$]:

$$\begin{aligned}
\frac{\partial B}{\partial X} &= \frac{1}{R} \frac{\partial B}{\partial \alpha} \\
\frac{\partial B}{\partial Y} &= \frac{\partial B}{\partial R} \\
\frac{\partial^2 B}{\partial X^2} &= \frac{1}{R^2} \frac{\partial^2 B}{\partial \alpha^2} + \frac{1}{R} \frac{\partial B}{\partial R} \\
\frac{\partial^2 B}{\partial X \partial Y} &= \frac{1}{R} \frac{\partial^2 B}{\partial \alpha \partial R} - \frac{1}{R^2} \frac{\partial B}{\partial \alpha} \\
\frac{\partial^2 B}{\partial Y^2} &= \frac{\partial^2 B}{\partial R^2} \\
\frac{\partial^3 B}{\partial X^3} &= \frac{3}{R^2} \frac{\partial^2 B}{\partial \alpha \partial R} - \frac{2}{R^3} \frac{\partial B}{\partial \alpha} \\
\frac{\partial^3 B}{\partial X^2 \partial Y} &= \frac{-2}{R^3} \frac{\partial^2 B}{\partial \alpha^2} - \frac{1}{R^2} \frac{\partial B}{\partial R} + \frac{1}{R} \frac{\partial^2 B}{\partial R^2} \\
\frac{\partial^3 B}{\partial X \partial Y^2} &= \frac{2}{R^3} \frac{\partial B}{\partial \alpha} - \frac{2}{R^2} \frac{\partial^2 B}{\partial \alpha \partial R} \\
\frac{\partial^3 B}{\partial Y^3} &= 0 .
\end{aligned} \tag{3.2.7}$$

In fourth-order calculations the relations are the same up to second order, and then

$$\begin{aligned}
\frac{\partial^3 B}{\partial X^3} &= \frac{1}{R^3} \frac{\partial^3 B}{\partial \alpha^3} + \frac{3}{R^2} \frac{\partial^2 B}{\partial \alpha \partial R} - \frac{2}{R^3} \frac{\partial B}{\partial \alpha} \\
\frac{\partial^3 B}{\partial X^2 \partial Y} &= \frac{1}{R^2} \frac{\partial^3 B}{\partial \alpha^2 \partial R} - \frac{2}{R^3} \frac{\partial^2 B}{\partial \alpha^2} - \frac{1}{R^2} \frac{\partial B}{\partial R} + \frac{1}{R} \frac{\partial^2 B}{\partial R^2} \\
\frac{\partial^3 B}{\partial X \partial Y^2} &= \frac{1}{R} \frac{\partial^3 B}{\partial \alpha \partial R^2} + \frac{2}{R^3} \frac{\partial B}{\partial \alpha} - \frac{2}{R^2} \frac{\partial^2 B}{\partial \alpha \partial R} \\
\frac{\partial^3 B}{\partial Y^3} &= \frac{\partial^3 B}{\partial R^3} \\
\frac{\partial^4 B}{\partial X^4} &= \frac{1}{R^4} \frac{\partial^4 B}{\partial \alpha^4} - \frac{8}{R^4} \frac{\partial^2 B}{\partial \alpha^2} + \frac{6}{R^3} \frac{\partial^3 B}{\partial \alpha^2 \partial R} + \frac{3}{R^2} \frac{\partial^2 B}{\partial R^2} - \frac{3}{R^3} \frac{\partial B}{\partial R} \\
\frac{\partial^4 B}{\partial X^3 \partial Y} &= \frac{1}{R^3} \frac{\partial^4 B}{\partial \alpha^3 \partial R} - \frac{3}{R^4} \frac{\partial^3 B}{\partial \alpha^3} + \frac{3}{R^2} \frac{\partial^3 B}{\partial \alpha \partial R^2} - \frac{8}{R^3} \frac{\partial^2 B}{\partial \alpha \partial R} + \frac{6}{R^4} \frac{\partial B}{\partial \alpha} \\
\frac{\partial^4 B}{\partial X^2 \partial Y^2} &= \frac{1}{R^4} \frac{\partial^2 B}{\partial \alpha^2} - \frac{4}{R^3} \frac{\partial^3 B}{\partial \alpha^2 \partial R} - \frac{2}{R^2} \frac{\partial^2 B}{\partial R^2} + \frac{2}{R^3} \frac{\partial B}{\partial R} + \frac{1}{R^2} \frac{\partial^4 B}{\partial \alpha^2 \partial R^2} + \frac{1}{R} \frac{\partial^3 B}{\partial R^3} \\
\frac{\partial^4 B}{\partial X \partial Y^3} &= \frac{1}{R} \frac{\partial^4 B}{\partial \alpha \partial R^3} - \frac{3}{R^2} \frac{\partial^3 B}{\partial \alpha \partial R^2} + \frac{6}{R^3} \frac{\partial^2 B}{\partial \alpha \partial R} - \frac{6}{R^4} \frac{\partial^4 B}{\partial \alpha^4} \\
\frac{\partial^4 B}{\partial Y^4} &= \frac{\partial^4 B}{\partial R^4} .
\end{aligned} \tag{3.2.8}$$

Extrapolation from the median plane field $B_Z(X, Y, 0)$ to $\vec{B}(X, Y, Z)$

Median plane antisymmetry is assumed, which results in:

$$B_X(X, Y, 0) = 0$$

$$\begin{aligned}
B_Y(X, Y, 0) &= 0 \\
B_X(X, Y, Z) &= -B_X(X, Y, -Z) \\
B_Y(X, Y, Z) &= -B_Y(X, Y, -Z) \\
B_Z(X, Y, Z) &= B_Z(X, Y, -Z) .
\end{aligned}$$

Together with Maxwell's equations, out of the median plane this results in the following Taylor expansions, for the three components of $\vec{B}$ (here again B stands for $B_Z(X, Y, 0)$):

$$\begin{aligned}
B_X(X, Y, Z) &= Z \frac{\partial B}{\partial X} - \frac{Z^3}{6} \left(\frac{\partial^3 B}{\partial X^3} + \frac{\partial^3 B}{\partial X \partial Y^2} \right) \\
B_Y(X, Y, Z) &= Z \frac{\partial B}{\partial Y} - \frac{Z^3}{6} \left(\frac{\partial^3 B}{\partial X^2 \partial Y} + \frac{\partial^3 B}{\partial Y^3} \right) \\
B_Z(X, Y, Z) &= B - \frac{Z^2}{2} \left(\frac{\partial^2 B}{\partial X^2} + \frac{\partial^2 B}{\partial Y^2} \right) + \frac{Z^4}{24} \left(\frac{\partial^4 B}{\partial X^4} + 2 \frac{\partial^4 B}{\partial X^2 \partial Y^2} + \frac{\partial^4 B}{\partial Y^4} \right) .
\end{aligned} \tag{3.2.9}$$

which are then differentiated one by one with respect to X, Y , or Z , up to second or (optionally) fourth order, in order to get the expressions involved in Eq. (2.1.10).

3.3 MULTIPOL: Magnetic Multipole

The simulation of a multipolar field $\vec{M}$ by the MULTIPOL procedure proceeds by addition of the dipolar ($\vec{B}1$), quadupolar ($\vec{B}2$), sextupolar ($\vec{B}3$), octupolar ($\vec{B}4$), decapolar ($\vec{B}5$) and dodecapolar ($\vec{B}6$) transverse components, and of their derivatives up to fourth order. For instance,

$$\begin{aligned}
\vec{M} &= \vec{B}1 + \vec{B}2 + \vec{B}3 + \vec{B}4 + \vec{B}5 + \vec{B}6 \\
\frac{\partial \vec{M}}{\partial X} &= \frac{\partial \vec{B}1}{\partial X} + \frac{\partial \vec{B}2}{\partial X} + \frac{\partial \vec{B}3}{\partial X} + \frac{\partial \vec{B}4}{\partial X} + \frac{\partial \vec{B}5}{\partial X} + \frac{\partial \vec{B}6}{\partial X} \\
\frac{\partial^2 \vec{M}}{\partial X \partial Z} &= \frac{\partial^2 \vec{B}1}{\partial X \partial Z} + \frac{\partial^2 \vec{B}2}{\partial X \partial Z} + \frac{\partial^2 \vec{B}3}{\partial X \partial Z} + \frac{\partial^2 \vec{B}4}{\partial X \partial Z} + \frac{\partial^2 \vec{B}5}{\partial X \partial Z} + \frac{\partial^2 \vec{B}6}{\partial X \partial Z} . \\
&\text{etc...}
\end{aligned} \tag{3.3.1}$$

Entrance and exit longitudinal (X) fringe fields can be introduced. They are characterized by their extents at the entrance and exit of the magnet. Their fall-off model is the same as for the DIPOLE (Eq. 3.3.3 below and Fig. 10). The fringe fields are treated separately for each multipole component.

Any multipole component $\vec{B}_n$ can be X -rotated independently of the others by an arbitrary angle for the simulation of positioning defects, as well as skewed lenses.

The explicit expressions of the field and their derivatives $\partial^{i+j+k} \vec{B}_n / \partial X^i \partial Y^j \partial Z^k$ as involved in Eqs. (2.1.10), derive from the classical expression for the scalar potential [14]

$$V_n(X, Y, Z) = (n!)^2 \left(\sum_{q=0}^{\infty} (-1)^q \frac{G^{(2q)}(X) (Y^2 + Z^2)^q}{4^q q! (n+q)!} \right) \left(\sum_{m=0}^n \frac{\sin(m\frac{\pi}{2}) Y^{n-m} Z^m}{m! (n-m)!} \right) , \tag{3.3.2}$$

where $G(X)$ is the longitudinal gradient defined at the entrance or exit of the magnet by (S stands for the distance to the EFB)

$$G(S) = \frac{G_0}{1 + \exp(P(S))} \quad , \quad G_0 = \frac{B_0}{R_0^{n-1}} . \tag{3.3.3}$$

4 APPLICATION TO AN INVERSE PROBLEM: OPTIMIZATION OF QD SPECTROMETER

The set-up

Figure 12 shows the geometry of the spectrometer addressed. Details of the iso-magnetic lines of the dipole field map as generated by the DIPOLE procedure prior to ray-tracing, are displayed in Fig. 13. On top of it appear three sets of three rays each that correspond to the three momenta 600 (minimum), 750 (central) and 900 MeV/c. These momenta appear to be focused at three specific spots on the final focal surface of the spectrometer. The related input data file to ZGOUBI is given in Table 4.1.

Table 4.1: The input data file to ZGOUBI corresponding to Fig. 13

750 MeV/c QD spectrometer	Definition of the initial conditions
'OBJET'	Rigidity (namely, 750 MeV/c protons)
2501.73	
1	
1 3 1 1 3	To = +/- 50 mrad, and p = 600, 750, 1200 MeV/c
0. 50. .0 0. .1	
1.	
'ESL'	Drift space (cm)
60.	
'QUADRUPO'	Definition of the Quadrupole
0	
80. 15. -7.6	Length (cm), radius (cm), field (kG)
25. 30.	Definition of the entrance fringe field
6 .1122 6.2671 -1.4982 3.5882 -2.1209 1.723	
25. 30.	Definition of the exit fringe field
6 .1122 6.2671 -1.4982 3.5882 -2.1209 1.723	
4.	Integration step size (cm)
1 0. 0. 0.	
'ESL'	Drift space (cm)
9.32978	
'CHANGREF'	Positioning of the next optical element
0. 0. 19.	in the current referential
'DIPOLE'	Definition of the Dipole
2 0 0	
350 200	350 times 200 nodes map mesh
17 0. 0. 0.	Field (kG)
102. 41.5 147.16 97.157 247.157	Angles and radii that limit the map
20. -1.	Definition of the entrance fringe field
4 .1455 2.2670 -.6395 1.1558 0. 0. 0.	and EFB (straight)
22.5 0. 1.E6 -1.E6 1.E6 1.E6	
20. -1.	Definition of the exit fringe field
4 .1455 2.2670 -.6395 1.1558 0. 0. 0.	and EFB (R1 = R2 = 525cm)
-22.5 41. 525 0. 0. 525	
0	
2	
4.9	Integration step size (cm)
2	
155.63946 0. 0. 0.	
'END'

Figure 12: A 750 MeV/c QD spectrometer. Momentum bite: 600–1200 MeV/c.

Figure 13: Detail of the isomagnetic lines of the dipole, from the field map as generated by the DIPOLE procedure prior to ray-tracing. Three sets of rays of, respectively, momenta 600, 750, and 900 MeV/c, have been ray-traced through the optical device, as plotted on top of the field map.

Optimizing the optical quality

We now apply the FIT procedure. A set of 11 particles with a central momentum of 750 MeV/c originating from a point object situated at the target, are launched in the horizontal plane with initial angles $-50 \leq T \leq 50$ mrad by 10 mrad steps (see Fig. 1 for the coordinates definition). Owing to the optical aberrations, the image (on the final focal surface) of this zero size point object has a non-zero size. The FIT procedure is used

for optimizing the two dipole exit face curvature values R_1 and R_2 [Fig. 9(a)], in order to compensate as much as possible the effect of the optical aberrations, i.e. with the goal of minimizing the size of the image that the 11 rays produce on the final focal surface.

Table 4.2 displays the corresponding input data file to ZGOUBI. The aberration curves in the horizontal phase plane (Y,T), prior and posterior to the fit procedure, are shown in Fig. 14. The FIT procedure required about 50 ‘calls to the function’ (namely, the number of times that the 11 rays have been ray-traced through the optical structure), and an execution time of about one minute on an HP workstation.

Table 4.2: Input data file for the fit of the exit face curvatures

750 MeV/c QD spectrometer. 'OBJET' 2501.73 2 13 1 0. -50. .0 0. 1. 'o' 0. -40. .0 0. 1. 's' 0. -30. .0 0. 1. 's' 0. -20. .0 0. 1. 's' 0. -10. .0 0. 1. 's' 0. -1. .0 0. 1. 'a' 0. 0. .0 0. 1. 's' 0. 1. .0 0. 1. 'a' 0. 10. .0 0. 1. 's' 0. 20. .0 0. 1. 's' 0. 30. .0 0. 1. 's' 0. 40. .0 0. 1. 's' 0. 50. .0 0. 1. 's' 1 1 1 1 1 1 1 1 1 1 1 1 'ESL' 60. 'QUADRUPO' 0 80. 15. -7.6 25. 30. 6 .1122 6.2671 -1.4982 3.5882 -2.1209 1.723 25. 30. 6 .1122 6.2671 -1.4982 3.5882 -2.1209 1.723 4. 1 0. 0. 0. 'CHANGREF' 9.32978. 0. 19. 'DIPOLE' 2 0 0 350 200 17 0. 0. 0. 102. 41.5 147.16 97.157 247.157 20. -1. 4 .1455 2.2670 -.6395 1.1558 0. 0. 0. 22.5 0. 1.E6 -1.E6 1.E6 1.E6 20. -1. 4 .1455 2.2670 -.6395 1.1558 0. 0. 0. -22.5 41. 525 0. 0. 525 0 2 4.9 2 155.63946 0. 0. 0. 'AUTOREF' 3 7 6 8 'FIT' 2 5 43 0 .8 5 46 0 .8 1 0 1 1 6 0. 1. 'END'	Definition of the initial conditions Rigidity (namely, 750 MeV/c protons) 13 trajectories to be ray-traced Yo, To, Zo, Po, dp/p, tagging letter (To = horizontal angle) Drift space (cm) Definition of the Quadrupole Length (cm), radius (cm), field (kG) Definition of the entrance fringe field Definition of the exit fringe field Integration step size (cm) Positioning of the next optical element in the current referential Definition of the Dipole 350 times 200 nodes map mesh Field (kG) Angles and radii that limit the map Definition of the entrance EFB (straight) and fringe field Definition of the exit EFB (R1 = R2 = 525cm) and fringe field Integration step size (cm) Defines the position of the final transverse plane (at intersection of rays 7, 6 and 8) Minimize the image size in the final transverse plane 2 variables: R1 (parameter #43 of element #5-DIPOLE) R2 (parameter #46 of element #5) 1 constraint, after element #6-AUTOREF coefficient [1,1] of the beam matrix; value = 0
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Figure 14: Aberration curves in the horizontal phase plane (Y , T), at the focal surface. (a) Before the fit of the exit face curvatures R_1 and R_2 . The initial values of the two variables are $R_1 = R_2 = 5.25$ m. (b) After the fit of the exit faces curvatures R_1 and R_2 . The final values of the two variables are $R_1 = 4.81$ m and $R_2 = 4.59$ m. It can be observed that their fitting has resulted in an appreciable decrease of the distortion of the aberration curve, and hence of the size of the image on the focal surface, for the particular momentum of concern, 750 MeV/c. (c) Another example of initial (to low) values $R_1 = R_2 = 4.25$ m.

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