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IGUN to OPTR for ECR

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Abstract: The purpose two-fold: (1) to clarify the use of the IGUN output for application in TRANSOPTR, and (2) to indicate how the beam can be modelled from rest inside the ECR ion source.

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1 Introduction

Ions created inside an axial magnetic field have polar coordinates (r, r', θ, θ'). We are not interested in the longitudinal motion at this point and beam is cw with minimal energy spread. IGUN[1] outputs particle coordinates, omitting the θ coordinate. This is possible for axially symmetric sources and makes the simulation highly efficient. Thus each "particle" in fact represents all azimuths and can be thought of as a ring of particles. The population of the ring is given as a separate output as a current labelled `Ampere`.

Nevertheless the rings have an azimuthal speed $r\theta'$ labelled `ATAN(DT/DZ)`. (This is meant to stand for $\arctan(r\theta')$ but as it is always $\ll 1$, we can ignore the arctan.) In fact, it is a characteristic of ECR sources that the average azimuthal rate of rotation is not zero; i.e. the beam exits the source spinning about the axis. This is due to the ECR's magnetic field.

The remaining two coordinates r, r' are labelled `RHO` (mm) and `ATAN(DR/DZ)`. The final z-coordinate is for some unaccountable reason labelled `ZETA`. The kinetic energy per charge is `Etot/Q` in volts. The only other columns of interest are the mass and charge numbers, labelled appropriately.

From the symmetry, we can calculate the beam's second moments as follows. Since

$$x = r\cos\theta,\ \ y = r\sin\theta, \tag{1}$$

we have

$$x' = r'\cos\theta - r\theta'\sin\theta,\ \ y' = r'\sin\theta + r\theta'\cos\theta. \tag{2}$$

Thus knowing the uniform distribution of angles, we (the 'student') can show the following for the beam's second moments:

$$\langle x^2\rangle = \langle y^2\rangle = \langle r^2\rangle/2, \tag{3}$$

$$\langle xx'\rangle = \langle yy'\rangle = \langle rr'\rangle/2, \tag{4}$$

$$\langle x'^2\rangle = \langle y'^2\rangle = \langle r'^2\rangle/2 + \langle (r\theta')^2\rangle/2. \tag{5}$$

The square of the rms emittance is thus

$$\epsilon_x^2 = \epsilon_y^2 = \langle x^2\rangle\langle x'^2\rangle - \langle xx'\rangle^2 = [\langle r^2\rangle\langle r'^2\rangle - \langle rr'\rangle^2 + \langle r^2\rangle\langle (r\theta')^2\rangle]/4. \tag{6}$$

But there are further correlations if the beam is rotating about the axis due to the magnetic field:

$$\langle xy\rangle = 0,\ \ \langle x'y'\rangle = 0, \tag{7}$$

but

$$\langle xy'\rangle = -\langle x'y\rangle = \langle r^2\theta'\rangle/2. \tag{8}$$

For use in `TRANSOPTR`, there are only four independent parameters and the beam sigma matrix has the following form.

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 & \sigma_{14} \\ \sigma_{12} & \sigma_{22} & -\sigma_{14} & 0 \\ 0 & -\sigma_{14} & \sigma_{11} & \sigma_{12} \\ \sigma_{14} & 0 & \sigma_{12} & \sigma_{22} \end{pmatrix} \tag{9}$$

If the coupling correlation is ignored, one finds the transverse emittances as usual as

$$\epsilon_x = \epsilon_y = \sqrt{\sigma_{11}\sigma_{22} - \sigma_{12}^2}, \tag{10}$$

the square root of the 2D determinant. But the actual 4D emittance is not the product of x and y emittances but rather this determinant gives

$$\epsilon_{4D} = \sigma_{11}\sigma_{22} - \sigma_{12}^2 - \sigma_{14}^2 \tag{11}$$

To understand this more deeply, let us assume a completely uncoupled axially symmetric beam,

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 & 0 \\ \sigma_{12} & \sigma_{22} & 0 & 0 \\ 0 & 0 & \sigma_{11} & \sigma_{12} \\ 0 & 0 & \sigma_{12} & \sigma_{22} \end{pmatrix} \tag{12}$$

The canonical momenta include a component due to the vector potential, which to good approximation has only an azimuthal component $A_\theta = \frac{1}{2}B_0(z)r$, or $A_x = \frac{-y}{2}B_0, A_y = \frac{x}{2}B_0$. the changes to x' and y' are these components multiplied by charge and divided by the reference momentum, and since $mv/q = B\rho$, we have that $\Delta x' = -\frac{y}{2\rho}, \Delta y' = \frac{x}{2\rho}$, or the transfer matrix is

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -\kappa & 0 \\ 0 & 0 & 1 & 0 \\ \kappa & 0 & 0 & 1 \end{pmatrix}, \tag{13}$$

where $\kappa := \frac{-B}{2B\rho} = \frac{-1}{2\rho}$. Applied to the uncorrelated sigma matrix as $\Sigma_{ECR} = M\Sigma M^{\mathrm{T}}$, we get

$$\Sigma_{ECR} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 & \kappa\sigma_{11} \\ \sigma_{12} & \kappa^2\sigma_{11} + \sigma_{22} & -\kappa\sigma_{11} & 0 \\ 0 & -\kappa\sigma_{11} & \sigma_{11} & \sigma_{12} \\ \kappa\sigma_{11} & 0 & \sigma_{12} & \kappa^2\sigma_{11} + \sigma_{22} \end{pmatrix}. \tag{14}$$

Now the emittance of one plane is

$$\sigma_{11}\sigma_{22} + \kappa^2\sigma_{11}^2 - \sigma_{12}^2, \tag{15}$$

This clarifies that the effect of the axial field is to augment the emittance, with an additional component of

$$\Delta\epsilon_x = \kappa\sigma_{11} = \frac{r^2}{2\rho} \quad (16)$$

added to the uncorrelated emittance. (It's actually added in quadrature, so the left side should read $\sqrt{\Delta\epsilon_x^2}$.) Taking the 4×4 determinant, we find the 4D emittance is unchanged at

$$\epsilon_{4D} = \sigma_{11}\sigma_{22} - \sigma_{12}^2, \quad (17)$$

and Liouville theorem still holds (the larger 22 element cancels the coupling component), but all 2D projections display the larger emittance.

2 Modelling in `TRANSOPTR`

`TRANSOPTR` can correctly model the linear optics of a varying axial magnetic field. It does so using canonical momenta: instead of tracking (x', y'), it tracks (P_x, P_y). This has the advantage that there are no entry and exit matrices to the field region.[2] The canonical momenta are related to the kinetic momenta (p_x, p_y) by

$$\vec{P} = \vec{p} + q\vec{A}, \quad (18)$$

where $\vec{A}$ is the vector potential, which to first order in an axially symmetric magnetic field is simply

$$\vec{A} = \frac{B(s)}{2}(-y, x, 0). \quad (19)$$

The magnetic field in first order is thus

$$\vec{B} = \nabla \times \vec{A} = \left(-\frac{B'}{2}x, \frac{B'}{2}y, B\right), \quad (20)$$

or, in other words, the axial field plus a radial field that is linear and given by half the derivative of the axial field. If we were to track particles or beam distributions through this field we could do it by applying the Lorentz force law $\vec{F} = q\vec{v} \times \vec{B}$.

But this is not the way `TRANSOPTR` does it. Instead, using canonical momenta, the Hamiltonian is

$$H = \frac{p_x^2}{2} + \frac{p_y^2}{2} = \frac{1}{2}(P_x + \kappa y)^2 + \frac{1}{2}(P_y - \kappa x)^2.^1 \quad (21)$$

[1] Note that for simplicity, we scale all momenta by the beam's reference momentum, as this makes in field-free regions for example $x' = p_x$.

The resulting equations of motion are

$$x' = \frac{\partial H}{\partial P_x} = P_x + \kappa y \tag{22}$$
$$P_x' = -\frac{\partial H}{\partial x} = -\kappa^2 x + \kappa P_y \tag{23}$$
$$y' = \frac{\partial H}{\partial P_y} = P_y - \kappa x \tag{24}$$
$$P_y' = -\frac{\partial H}{\partial y} = -\kappa^2 y - \kappa P_x, \tag{25}$$

and no differentiation of $B(s)$ is needed.

Simply integrating these equations is correct for any beam originating outside the axial field and passing through it. But for a beam **created** inside an axial field, such as is the case for an ECR ion source, the initial beam has to be corrected. Since `TRANSOPTR` assumes the initial given σ-matrix is canonical, the particles that originate e.g. from a Maxwell-Boltzmann initial momentum distribution, need to have their momenta corrected according to their position with respect to the axis. This is given by eqn.18, or,

$$P_x = x' - \kappa y \tag{26}$$
$$P_y = y' + \kappa x, \tag{27}$$

or in other words, by applying the matrix eqn. 13. This is handled in `TRANSOPTR` by a call to the routine `TMAT` as the first call in the system routine `TSYSTEM`.

This starting beam raises an interesting problem that had to be resolved. When integrating in mode 4 or 5, the numerical Runge-Kutta error is found from a symplectic check, and it is compared with the set error tolerance specified in `data.dat`. However, the matrix in eqn. 13 is flagrantly non-symplectic: $M_{11}M_{23} - M_{13}M_{21} + M_{31}M_{43} - M_{33}M_{41}$ should be zero but is actually -2κ, and this symplectic error is invariant through the remainder of the symplectic transport elements. It makes ineffective the error checking. This was resolved by adding a symplectic check to `TMAT`, and inhibiting the application of the matrix to the accumulated transfer matrix while still allowing its application to the accumulating σ-matrix.

References

[1] R. Becker, W. B. Herrmannsfeldt, `IGUN` - A program for the simulation of positive ion extraction including magnetic fields, Review of Scientific Instruments 63 (4) (1992) 2756–2758. `doi:10.1063/1.1142795`.

[2] R. Baartman, End Effects of Beam Transport Elements, talk at Snowmass (July 2001).
URL `http://lin12.triumf.ca/text/Talks/2001Snowmass/FF.pdf`