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F. Antonangeli and M. Piacentini:
RAY TRACING CALCULATION FOR THE PULS FACILITY

PART II: THE THREE-DIMENSIONAL CASE

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# RAY TRACING CALCULATION FOR THE PULS FACILITY

## PART II: THE THREE-DIMENSIONAL CASE

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## 1. - INTRODUCTION

Ray tracing is the best method for studying the imaging properties of an optical system. By applying the laws of reflection or refraction at each optical surface of the system, one can follow each ray from the source to its image. The imaging properties of the system can be visualized easily by calculating the cross section of the beam, i.e. the intersection of each ray with a plane perpendicular to the beam at any desired position along the system. By changing the parameters of the system, the variation of the image can be followed and the image itself can be optimized. However, this is a rather difficult task, that requires a good deal of computer time.

The technique for ray tracing calculations is well known and described in detail in several textbooks(1). Applications to special problems, such as the combination of a toroidal mirror with a spherical grating operating at grazing incidence, are also well known(2).

In order to study the optical system designed for the PULS facility constructed at the storage ring ADONE of the INFN National Laboratories in Frascati(3), we have written a ray tracing program, that includes the choice between toroidal, cylindrical, and spherical mirrors. In the first report on this series, hereafter referred to as R1(4), we have given the formulation for the ray tracing in the meridian plane of a mirror of circular section. We have shown that a power expansion of the ray tracing equations in the variable $\theta$, the beam divergence, gives an accurate description of the imaging properties of the mirror.

In this report we shall extend the formulation of R1 to the three-dimensional case. In Sect. 2 we give the general expressions, written explicitely in analytical form. In Sect. 3 we apply them to a toroidal and a flat mirror in detail, and give the basic equations for cylindrical and spherical mirrors. In Sect. 4 we give a brief description of the ray tracing program and an example of its application. In the third report of this series we shall expand the ray tracing equations in power series of $\theta$, $\varphi$, the beam divergences, and $\eta$, $\zeta$, the source dimensions, that are small compared with the distance of the source from the mirror.

## 2. - GENERAL FORMULATION

The optical system that we shall study is shown in Fig. 1. The center of the mirror, formed by a revolution surface with the concavity facing upwards, is in the origin of the coordinate system $\Sigma(x, y, z)$. The meridian

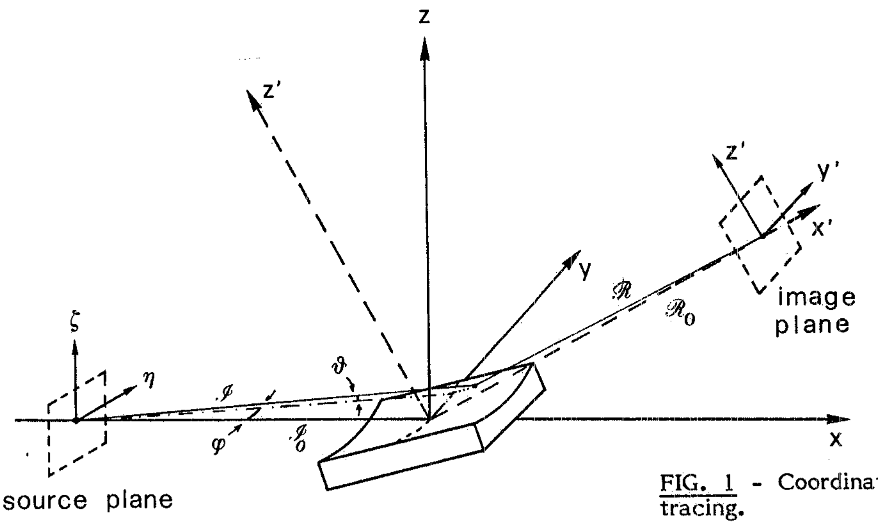


FIG. 1 - Coordinates and notations for the ray tracing.

plane of the mirror is the xz plane. With this choice, by setting y=0, we must recover the equations of R1. The incidence central ray $\mathcal{I}_0$ is coincident with the negative portion of the x axis, the source being located in $S=(-s,\eta,\zeta)$. The tangential angle of incidence(*) of the central ray with the mirror is $i_0$. The reflected central ray $\mathcal{R}_0$ is directed upwards in the upper half meridian plane and forms an angle $r_0=2i_0$ with the x axis. In order to find the imaging properties of the mirror after the reflection, we shall rotate the coordinate system $\Sigma$ around the y axis by the angle $r_0$, so that the x axis of the new coordinate system $\Sigma'(x', y', z')$ is coincident with $\mathcal{R}_0$. The aim of the ray tracing method is to find the intersections $Q(x', y', z')$ of the reflected rays with planes perpendicular to $\mathcal{R}_0$, that give the cross sections of the reflected beam. Once the parameters of the rays reflected by the mirror are known, they can be used as input parameters for the next mirror. The coordinates of Q cannot be derived analytically, but must be obtained numerically following several steps as described below.

If we represent the surface $\Omega$ of the mirror by the equation

$$F(x, y, z) = 0 , \tag{1}$$

the coordinates of the point $P(x_c, y_c, z_c)$ of intersection between the surface $\Omega$ and the rays $\mathcal{I}$ leaving the source are obtained by solving the system of equations:

$$\begin{cases} F(x, y, z) = 0 , & \text{(1a)} \\ \dfrac{z-\zeta}{n_i} = \dfrac{x+s}{l_i} , & \text{(2a)} \\ \dfrac{y-\eta}{m_i} = \dfrac{x+s}{l_i} . & \text{(2b)} \end{cases}$$

---

(*) Throughout this report we shall use for convenience the tangential angle of incidence between the incident rays and the plane tangent to the mirror, rather than the conventional angle of incidence between the incident rays and the normal to the surface. In soft X-ray and X-ray optics, the tangential angle of incidence is small (grazing incidence).

Eqs. (2) are the equations of a straight line passing through S and with direction cosines $(l_i, m_i, n_i)^{(+)}$.

We can express the direction cosines in terms of the polar angular coordinates $\theta$ and $\varphi$ referred to the x axis, as indicated in Fig. 1:

$$l_i = \cos\theta\cos\varphi\ ,$$
$$m_i = \cos\theta\sin\varphi\ , \qquad (3)$$
$$n_i = \sin\theta\ .$$

Here $\theta$ is the divergence of the rays in the meridian plane and has the same meaning as in R1. $\varphi$ is the sagittal divergence in a plane normal to the meridian plane.

The tangent angle of incidence i for the incident rays is given by:

$$\sin i = \left| l_i l_n + m_i m_n + n_i n_i \right| , \qquad (4)$$

where

$$l_n = \varrho \left.\frac{\partial F}{\partial x}\right|_P \ ,$$
$$m_n = \varrho \left.\frac{\partial F}{\partial y}\right|_P \ , \qquad (5)$$
$$n_n = \varrho \left.\frac{\partial F}{\partial z}\right|_P$$

are the direction cosines of the normal $\mathcal{N}$ to $\Omega$ in P, and

$$\varrho = \pm \left[ \left(\frac{\partial F}{\partial x}\right)_P^2 + \left(\frac{\partial F}{\partial y}\right)_P^2 + \left(\frac{\partial F}{\partial z}\right)_P^2 \right]^{-1/2}$$

is a normalization factor. The sign of $\varrho$ must be chosen so as to orienting $\mathcal{N}$ towards the concavity of the mirror and, consequently, $l_n < 0$. We recall here that the normal to the surface $\Omega$ is defined as the line perpendicular to the plane $\pi_t$ tangent to $\Omega$ in P. The equation of $\pi_t$ is given by

$$l_n(x-x_c) + m_n(y-y_c) + n_n(z-z_c) = 0. \qquad (6)$$

We introduce also the plane of incidence $\pi_i$ defined as the plane containing both $\mathcal{I}$ and $\mathcal{N}$, of equation

$$a_i(x-x_c) + b_i(y-y_c) + c_i(z-z_c) = 0, \qquad (7)$$

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(+) Hereafter we shall consider only normalized direction cosines: $l_i^2+m_i^2+n_i^2=1$.

with

$$a_i = m_n n_i - m_i n_n \quad ,$$
$$b_i = n_n l_i - l_n n_i \quad , \qquad (8)$$
$$c_i = l_n m_i - m_n l_i ,$$
$$a_i^2 + b_i^2 + c_i^2 = \cos^2 i .$$

From Eq. (4), the tangent angle is limited between 0° and 90°. However, the scalar product $l_i l_n + m_i m_n + n_i n_n$ in general can be either positive or negative. For the central ray it equals $l_n$ and it is negative. For continuity, for a concave reflectiving surface of small dimensions, $l_i l_n + m_i m_n + n_i n_n$ will be negative for all the incident rays, and Eq. (4) can be rewritten as

$$\sin i = -(l_i l_n + m_i m_n + n_i n_n) \qquad (4a)$$

The direction cosines of the reflected rays $\mathcal{R}$ are obtained by imposing the laws of reflection: i) $\mathcal{R}$ lies on $\pi_i$ and ii) the angle of reflection is equal to the angle of incidence. By imposing the third condition of normalization and with the help of Eq. (4a), we obtain:

$$l_r = l_i + 2 l_n \sin i \quad ,$$
$$m_r = m_i + 2 m_n \sin i \quad , \qquad (9)$$
$$n_r = n_i + 2 n_n \sin i \quad .$$

Now we have all the ingredients for writing the equations of the reflected rays $\mathcal{R}$:

$$\frac{y - y_c}{m_r} = \frac{x - x_c}{l_r} \quad ,$$
$$\qquad (10)$$
$$\frac{z - z_c}{n_r} = \frac{x - x_c}{l_r} \quad .$$

The rotation of the coordinate system by an angle $r_o$ around the y axis, given by the unitary matrix

| | x | y | z |
|---|---|---|---|
| x' | $\cos r_o$ | 0 | $\sin r_o$ |
| y' | 0 | 1 | 0 |
| z' | $-\sin r_o$ | 0 | $\cos r_o$ |

brings Eqs. (10) into:

$$y' = y_c + \frac{m_r}{n_r \sin r_o + l_r \cos r_o} (x' - x_c \cos r_o - z_c \sin r_o) \quad ,$$

$$z' = \frac{n_r \cos r_o - l_r \sin r_o}{n_r \sin r_o + l_r \cos r_o} ( x' - x_c \cos r_o - z_c \sin r_o) + z_c \cos r_o - x_c \sin r_o \quad , \tag{11}$$

and the reflected rays have direction cosines:

$$l'_r = n_r \sin r_o + l_r \cos r_o \quad ,$$

$$m'_r = m_r \quad , \tag{12}$$

$$n'_r = n_r \cos r_o - l_r \sin r_o .$$

As said at the beginning of this sections, the aim of the ray tracing method is to calculate the coordinates y' and z' at several distances x' from the mirror for all the rays leaving the source, in order to have the cross section of the reflected beam. In addition to give the shape of the reflected beam, the number of reflected rays, each of them multiplied by a proper intensity factor, falling per unit area of the cross section yields the distribution of the intensity at the image.

## 3. - APPLICATIONS TO SPECIAL CASES

### 3.1. - Flat Mirror

This case can be solved analytically to the end and it is helpful to check the procedures adopted. The equation of the flat mirror is:

$$x \sin i_o - z \cos i_o = 0 \quad . \tag{13}$$

The coordinates of P are given by

$$x_c = z_c \operatorname{ctg} i_o \quad ,$$

$$y_c = \frac{m_i}{l_i} \operatorname{ctg} i_o \, z_c + \frac{m_i}{l_i} \, s + \eta \, , \tag{14}$$

$$z_c = \left( \frac{n_i}{l_i} \, s + \zeta \right) \left(1 - \frac{n_i}{l_i} \operatorname{ctg} i_o\right)^{-1} \quad .$$

The normals to the flat surface are parallel to each other, indipendently from where they are drawn. In fact:

$$l_n = -\sin i_o \ ,$$

$$m_n = 0 \ , \qquad (15)$$

$$n_n = \cos i_o \ .$$

The angle of incidence is easily obtained from Eq. (4a):

$$\sin i = \sin i_o \, l_i - \cos i_o \, n_i \ . \qquad (16)$$

The direction cosines of the reflected rays are given by Eqs. (9) and (16)

$$l_r = l_i \cos 2 i_o + n_i \sin 2 i_o \ ,$$

$$m_r = m_i \ , \qquad (17)$$

$$n_r = l_i \sin 2 i_o - n_i \cos 2 i_o \ .$$

In the rotated reference frame $\Sigma'$ the direction cosines of the reflected rays become, following Eq. (12)

$$l'_r = l_i \ ,$$

$$m'_r = m_i \ , \qquad (18)$$

$$n'_r = -n_i \ ,$$

that are the same as the direction cosines of the incident rays. The cross section of the reflected beam at a distance x' from the mirror is easily obtained from Eqs. (11) using Eqs. (14), (17) and (18):

$$y' = \frac{m_i}{l_i} (x' + s) + \eta ,$$

$$z' = - \frac{n_i}{l_i} (x' + s) - \zeta . \qquad (19)$$

These equations correspond to the cross section of a not deflected beam at a distance s + x' from the source, with the exception of the change of sign of $n'_r$, and consequently of z', that corresponds to the right-left inversion of flat mirrors.

## 3.2. - Toroidal Mirror

Let us consider a toroidal mirror of radii of curvature R and r in the meridian and in the sagittal planes, respectively. For special values of R and r other shapes can be derived:

1) R = r the toroid reduces to a sphere

2) $r \to \infty$ the mirror is cylindrical, curved in the meridian plane, with generating lines parallel to the y axis.

3) $R \to \infty$ the mirror is cylindrical, curved in the sagittal plane, with generating lines parallel to the meridian plane.

4) $R \to \infty$ and $r \to \infty$ flat mirror.

The equation of the toroidal surface passing through the origin and oriented as shown in Fig. 1, is:

$$(x-\alpha)^2 + y^2 + (z-\gamma)^2 + (R-r)^2 - r^2 - 2\,(R-r)\sqrt{(x-\alpha)^2 + (z-\gamma)^2} = 0, \qquad (20)$$

with

$$\alpha = -R \sin i_o \;, \qquad \gamma = R \cos i_o \;. \qquad (21)$$

The intersection of a ray emitted by the source, given by Eqs. (2), and the toroidal surface (20) yields the following equation for $x_c$:

$$\frac{x_c^4}{l_i^4} - \frac{4\,x_c^3}{l_i^3}\,p + \frac{2\,x_c^2}{l_i^2}\left[2\,p^2 + q - 2\,(R-r)^2\,(l_i^2 + n_i^2)\right] - 4\,\frac{x_c}{l_i}\left[p\,q - 2\,(R-r)^2\,p'\right] + q^2 - 4\,(R-r)^2\,q' = 0. \qquad (22)$$

In the above equation p, q, p', and q' correspond to:

$$p = l_i\,\alpha - B_y\,m_i + \gamma'\,n_i,$$
$$q = \alpha^2 + B_y^2 + \gamma'^2 + (R-r)^2 - r^2,$$
$$p' = l_i\,\alpha + n_i\,\gamma',$$
$$q' = \alpha^2 + \gamma'^2 \;, \qquad (23)$$

respectively, and we have introduced

$$B_y = \frac{m_i}{l_i}\,s + \eta,$$
$$\gamma' = \gamma - B_z = \gamma - \frac{n_i}{l_i}\,s - \zeta. \qquad (24)$$

Eq. (22) has four solutions, corresponding to the four intersection points between a straight line and a torus. We have to choose the solution closest to the origin. It is possible that, due to the geometry of our problem, two solutions are complex, meaning that the rays $\mathcal{S}$ intersect only a portion of the torus. Once $x_c$ is known, through

Eqs. (2) also $y_c$ and $z_c$ can be calculated. From Eqs. (5) we have the direction cosines of $\mathcal{N}$:

$$l_n = \frac{x_c - \alpha}{r} \left[ \frac{R - r}{\sqrt{(x_c - \alpha)^2 + (z_c - \gamma)^2}} - 1 \right],$$

$$m_n = -\frac{y_c}{r} , \tag{25}$$

$$n_n = \frac{z_c - \gamma}{r} \left[ \frac{R - r}{\sqrt{(x_c - \alpha)^2 + (z_c - \gamma)^2}} - 1 \right] .$$

From this point we can write all the other expressions connected with the ray tracing, i.e. sin i and the reflected rays in the rotated reference frame $\Sigma$ '. Since we cannot solve analytically Eq. (22), such expressions result in long equations containing all the parameters defined above. In doing so we do not gain any further insight in the ray tracing equations that, instead, can be solved numerically easily. Also for the other types of surfaces discussed below we shall derive explicitely only $l_n$, $m_n$ and $n_n$.

### 3.3. - Spherical Mirror

The equation of a sphere with center on the xz plane and radius R, passing through the origin of the coordinate system, is :

$$(x - \alpha)^2 + y^2 + (z - \gamma)^2 = R^2 \tag{26}$$

where, as in Eq. (21), $\alpha$=-R sen $i_o$, $\gamma$ =R cos $i_o$, and $\alpha^2+\gamma^2-R^2=0$. This equation is easily obtained from Eq. (20) by putting r=R. One can apply all the equations given in Sect. 2 for obtaining the proper formulas for a spherical mirror, but it is more convenient to take the Eqs. of Sect. 3.2 and put r=R. $x_c$ is given by

$$x_c = l_i \left[ p - \sqrt{p^2 - q} \right] , \tag{27}$$

where p and q have the same meaning as in Eqs. (23). The direction cosines of the normals to the spherical surface are

$$l_n = -\frac{x_c - \alpha}{R} ,$$

$$m_n = -\frac{y_c}{R} , \tag{28}$$

$$n_n = -\frac{z_c - \gamma}{R} .$$

### 3.4. - Cylindrical mirrors

a) Generating lines parallel to the y axis ; curvature in the meridian plane. The equation corresponding to this mirror is

$$(x-\alpha)^2 + (z-\gamma)^2 - R^2 = 0, \tag{29}$$

with the condition $\alpha^2 + \gamma^2 - R^2 = 0$. $\alpha$ and $\gamma$ are given by Eq. (21). $x_c$ is given by:

$$x_c = \frac{l_i}{1-m_i^2}\left[(\alpha l_i + \gamma' n_i) - \sqrt{(\alpha l_i + \gamma' n_i)^2 - (1-m_i^2)(\alpha^2 + \gamma'^2 - R^2)}\right], \tag{30}$$

where $\gamma' = \gamma - \frac{n_i}{l_i} s - \zeta$ as in Eq. (24).

The direction cosines of the normal are:

$$l_n = -\frac{x_c - \alpha}{R}, \quad m_n = 0, \quad n_n = -\frac{z_c - \gamma}{R}. \tag{31}$$

b) Generating lines parallel to the x axis; curvature in the sagittal plane. The equation for this mirror is:

$$x^2 \sin^2 i_o + y^2 + z^2 \cos^2 i_o + 2 \sin i_o\, r\, x - 2 \cos i_o\, r\, z - 2 \cos i_o \sin i_o\, xz = 0 \tag{32}$$

$x_c$ is given by

$$x_c = \frac{l_i}{(n_i \cos i_o - l_i \sin i_o)^2 + m_i^2}\left[ (n_i \cos i_o - l_i \sin i_o)(r - B_z \cos i_o) - m_i B_y \right] + \sqrt{\left[m_i^2 + (n_i \cos i_o - l_i \sin i_o)^2\right] r^2 - \left[m_i (r - B_z \cos i_o) + B_y (n_i \cos i_o - l_i \sin i_o)\right]^2}. \tag{33}$$

The direction cosines of the normal are:

$$l_n = \frac{\sin i_o}{r}(z_c \cos i_o - r - x_c \sin i_o), \quad m_n = -\frac{y_c}{r}, \quad n_n = -\frac{\cos i_o}{r}(z_c \cos i_o - r - x_c \sin i_o). \tag{34}$$

As before, the knowledge of $x_c$ and $l_n$, $m_n$, $n_n$ allows the calculation of the parameters of the reflected rays.

## 4. - DESCRIPTION OF THE RAY TRACING PROGRAM

The ray tracing program developed for the PULS facility uses the equations derived in the previous sections. Several options are available: choice of the reflection plane (horizontal or vertical); choice of the reflection direction (up or down; right or left); choice of the type of mirror.

The program has been written following a pencil of rays leaving the source from the point $(-s, \eta, \zeta)$ all the way through the optical system. The program goes through a sequence of steps, that correspond to the logical steps described in Sect. 2:

1) Construction of the parameters of the pencil of rays. For each point of the source, a pencil of rays is defined by means of a set of equally spaced values of the two angles $\theta$ and $\varphi$, such that $|\theta_i| \leq \theta_M$ and $|\varphi_i| \leq \varphi_M$. $\theta_M$ and $\varphi_M$ correspond to the maximum half amplitudes of the radiation beam collected by the optical system.

2) Calculation of the coordinates $x_c$, $y_c$, and $z_c$ of intersection of the rays with the mirror, of the direction cosines of the normal, and of the direction cosines of the reflected rays. This step is performed by choosing among several "mirror type" subroutines. Each subroutine contains the equations given in Sect. 3 corresponding to a particular type of mirror. Since the equations have been determined for vertical, upwards reflection, the proper modifications have been introduced to take care of the other options on the direction of reflection.

3) Calculation of the parameters of the reflected rays in the rotated coordinate system $\Sigma'$.

4) Calculation of the cross section of the reflected beam at several distances from the mirror, corresponding to the intersection of each ray with planes perpendicular to the reflected central ray. The values of y' and z' are printed for each ray with the two values $\theta_i$ and $\varphi_i$ that define the original ray.

5) If the beam goes to another mirror, the parameters given in step 3), corrected for the shift of the coordinates origin along the x' axis to the center of the second mirror, are used as input parameters for a new calculation beginning from step 2). Note that in the program each ray is labelled with the original angular coordinates $\theta_i$ and $\varphi_i$ through the whole optical system.

In designing an optical system, it is important to allow for some adjustments necessary for positioning correctly all the optical components. Essentially, three tilts are necessary for a mirror, as shown in Fig. 2: i)

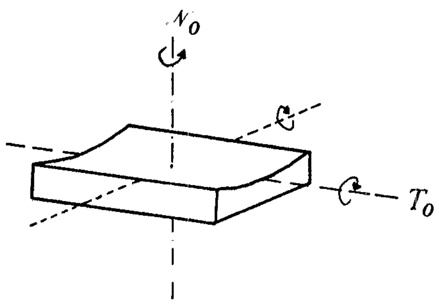


FIG. 2 - Tilts necessary to align a mirror in its ideal position.

rotation around the y axis to adjust $i_0$; ii) rotation around the tangent axis $T_0$ passing for the center of the mirror and perpendicular to the y axis, to bring the meridian plane into vertical position; iii) rotation around the normal $\mathcal{N}_0$ passing through the center of the mirror, in order to bring the two sections of circles corresponding to the two radii of curvature R and r parallel and perpendicular to the xz plane, respectively.

While positioning the mirror, it is useful to have a knowledge of the shape of the image of the source when the mirror is still misaligned, and to follow how the image changes while adjusting the mirror position. Our ray tracing program is written for the ideal case of perfect alignment. Equations for the mirrors, that include the tilted positions, can be used in the ray tracing program and the images of the source can be calculated as a function of the tilting parameters. However, this procedure requires expressions much more complicated than the ones used in the previous sections. Nevertheless, with our program we can perform the calculations for a misaligned mirror: it is enough to shift the source from its ideal position centered around $S_o(-s,0,0)$ to the proper position corresponding to the tilted situations. Accounting for a change of $i_o$ is straightforward. In the case ii), a positive rotation of the mirror by an angle $\psi$ around $T_o$ takes all the points $S(-s,\eta,\zeta)$ of the source into the positions $S'(s',\eta',\zeta')$ related to the old coordinates by

$$
\begin{aligned}
s' &= -s(\cos^2 i_o + \sin^2 i_o \cos\psi) + \eta \sin i_o \cos i_o (1-\cos\psi) + \eta \sin i_o \sin\psi ,\\
\eta' &= \eta \cos\psi + (s \sin i_o + \zeta \cos i_o) \sin\psi , \\
\zeta' &= s \sin i_o \cos i_o (\cos\psi - 1) - \eta \sin\psi \cos i_o + \zeta (\sin^2 i_o + \cos^2 i_o \cos\psi) .
\end{aligned}
\tag{35}
$$

Finally, in the case iii), a positive rotation of the mirror by an angle $\psi'$ around $\mathcal{N}_o$ corresponds to bringing the source into the position

$$
\begin{aligned}
s' &= -s(\sin^2 i_o + \cos^2 i_o \cos\psi') + \eta \cos i_o \sin\psi' +_{-} \zeta \sin i_o \cos i_o (\cos\psi' - 1),\\
\eta' &= (s \cos i_o - \zeta \sin i_o) \sin\psi' + \eta \cos\psi' , \\
\zeta' &= s \sin i_o \cos i_o (1 - \cos\psi') + \eta \sin i_o \sin\psi' + \zeta (\sin^2 i_o \cos\psi' + \cos^2 i_o).
\end{aligned}
\tag{36}
$$

Before concluding this report, in Fig. 3 we show the cross section of the radiation beam near the entrance slit of the monochromator Jobin Yvon LHT30 of the vacuum ultraviolet photoemission line, as calculated with the ray tracing program. The radiation, emitted by the electrons orbiting in Adone, is reflected in the vertical plane and focused in the meridian plane by the cylindrical mirror $S_I$ and then it is refocused on the entrance slit of the monochromator by a toroidal mirror in both the sagittal and the meridian planes. In Fig. 3 the calculated shape is compared also with a photograph of the beam.

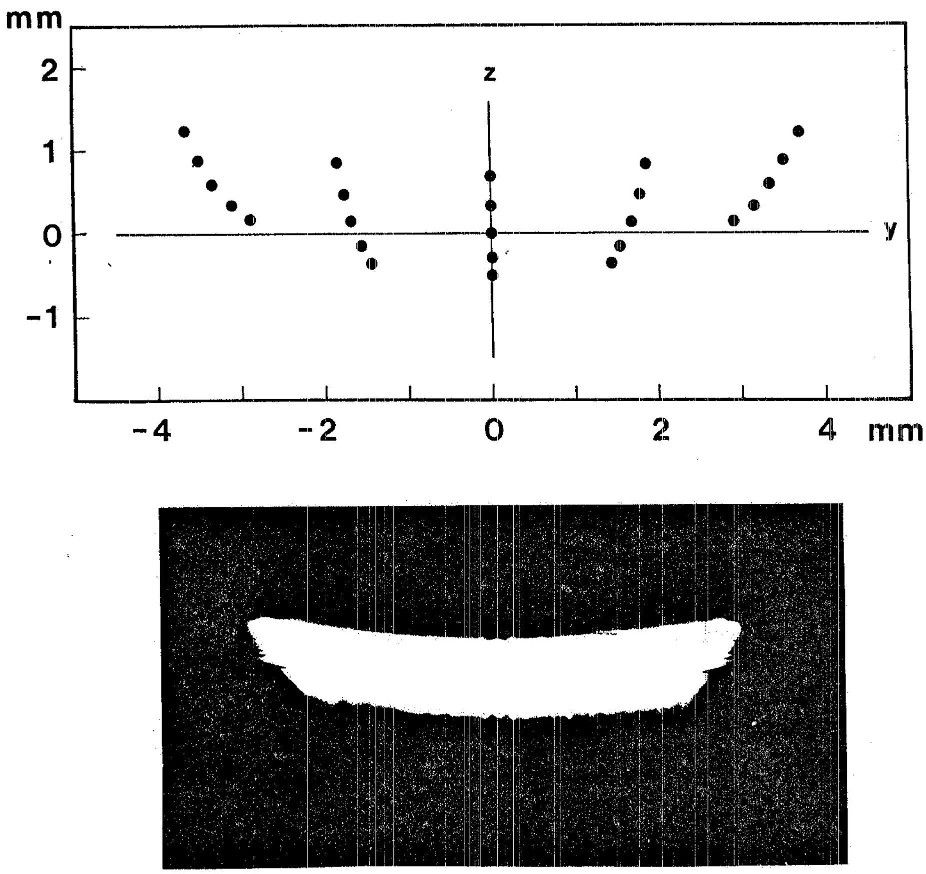


FIG. 3 - Calculated cross section of the synchrotron radiation beam near the entrance slit of the Jobin Yvon LHT30 monochromator, compared with a photograph of the beam, magnified ~ 7 times.

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