Statistical approach to beam shaping

Dmitry Varentsov,[1] Igor M. Tkachenko,[2] and Dieter H. H. Hoffmann[1,3]
[1]*Institut für Kernphysik, Technische Universität Darmstadt, Schlossgartenstraße 9, 64289 Darmstadt, Germany*
[2]*Departamento de Matemática Aplicada, Universidad Politécnica de Valencia, Camino de Vera s/n, 46022 Valencia, Spain*
[3]*Gesellschaft für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany*
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A method for beam shaping based on fitting the power moments of the final beam intensity distribution and independent of the optical system particularities is suggested. It is shown how one can analytically calculate any moment of the final phase space distribution using the moments of the initial distribution and the optical system transfer map. Numerical tests carried out for a final focus system have demonstrated the usefulness of the approach developed here.

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I. INTRODUCTION

By beam shaping we mean modification of the charged particle beam intensity distribution in the phase space at a point starting from a given input beam, in particular, producing an arbitrary transverse beam distribution after an optical transport channel. An important problem here is to provide a uniform target irradiation given a peaked (usually Gaussian) initial intensity distribution.

Beam shaping has many applications in science, industry, and medicine, such as spallation sources for isotope production and nuclear waist transmutation [1–5], proton and ion oncology [6,7], ion implantation, and material sciences. Other applications include minimization or/and control of beam halo in high-energy accelerators, colliders, transport lines, and final focus systems [8–11] to reduce beam loses and increase the acceptance of a system, to eliminate long collimation systems, or to increase the luminosity of a collider. Beam shaping is also essential for the high-energy density physics (HEDP) experiments with intense heavy ion beams [12–14].

Since the work of Meads [15], the concept of using nonlinear optical elements, such as octupoles and duodecapoles, for beam shaping has been developed in a number of analytical and numerical studies during the past 20 years [1–4,6,7,10,11,13,16,17]. The possibility of transverse shaping using octupoles has been also demonstrated experimentally [18]. Alternative approaches to beam shaping for particular cases not involving nonlinear optics, such as using a rf beam rotator or an exotic mode of a plasma lens operation, have also been proposed [19–21].

Unfortunately, existing analytical methods of beam shaping have only limited applicability for particular optical systems, low-order transfer maps, or certain shapes of initial or/and final distributions. These methods also have serious problems if momentum and geometrical coupling cannot be eliminated in a system or if the phase-space distribution of the beam at the positions of nonlinear elements is not flat.

In this paper we present a general approach to beam shaping based on analytical calculation of the power moments of the final distribution. In Sec. II it is shown how one can calculate the power moments of the final distribution if the transfer map of the optical system and the moments of the initial distribution are known. In Sec. III we discuss a possibility of beam shaping by fitting the final distribution moments. In Sec. IV examples of beam shaping calculations for a HEDP final focus system are presented.

II. POWER MOMENTS OF THE FINAL DISTRIBUTION

Let the coordinates of a particle at the entrance to an optical (shaping) system be $\mathbf{x}=\{x_1,x_2,\ldots,x_6\}$, where according to usual notation

$$x_1 = \mathrm{x}, \quad x_2 = \mathrm{a} = p_x/p_0,$$

$$x_3 = \mathrm{y}, \quad x_4 = \mathrm{b} = p_y/p_0,$$

$$x_5 = l, \quad x_6 = \delta_K. \tag{1}$$

These coordinates form three canonically conjugate pairs in which the transfer map is symplectic.

The initial phase-space distribution of the beam is given by the probability density function (PDF), $f(\mathbf{x})$. For the calculation examples presented in the paper we assume that *upstream* of the optical system the motion of the particles in transverse and longitudinal phase spaces is independent and the motion in the transverse (x_1,x_2) and (x_3,x_4) phase planes is decoupled as well

$$f(\mathbf{x}) = f_{12}(x_1,x_2)f_{34}(x_3,x_4)f_{56}(x_5,x_6). \tag{2}$$

Furthermore, we assume that f_{12}, f_{34}, and f_{56} are bivariate normal distribution functions of the corresponding coordinates,

$$f_{rt}(x_r,x_t) = \frac{1}{2\pi\epsilon_{rt}}\exp\left[-\frac{x_r^2\langle x_t^2\rangle - 2x_rx_t\langle x_rx_t\rangle + x_t^2\langle x_r^2\rangle}{2\epsilon_{rt}^2}\right], \tag{3}$$

where $\langle x_r^2\rangle=\sigma_r^2$, $\langle x_t^2\rangle=\sigma_t^2$ are the variances of the variables x_r and x_t, $\langle x_rx_t\rangle=\rho\sigma_r\sigma_t$ is the covariance and $\epsilon_{rt}=\sqrt{\langle x_r^2\rangle\langle x_t^2\rangle-\langle x_rx_t\rangle^2}$ is the rms emittance of the beam in the corresponding phase plane. The assumption of Eqs. (2) and (3) is certainly a limitation, though this ansatz is applicable to most of the systems of practical interest. It does not, however, reduce the generality of the method being suggested: the same theoretical approach can be applied to arbitrary initial beam intensity distribution in the six-dimensional phase space.

After passing through an optical system, the final coordinates of a particle are $\mathbf{X}=\{X_1,X_2\cdots X_6\}$ and the PDF of the beam is $F(\mathbf{X})$. The final coordinates $\mathbf{X}$ are related to initial coordinates $\mathbf{x}$ by a transfer map (Taylor expansion) $\mathcal{M}=\{\mathcal{M}_1,\mathcal{M}_2,\ldots,\mathcal{M}_6\}$

$$X_k=\mathcal{M}_k\circ\mathbf{x}=\sum_{\{i_s\},\Sigma i_s\leqslant N}\mathcal{M}_{k,\{i_s\}}x_1^{i_1}x_2^{i_2}\cdots x_6^{i_6}, \tag{4}$$

where N is the order of the transfer map. The elements $\mathcal{M}_{k,\{i_s\}}$ of the vectors $\mathcal{M}_k$ are proportional to the partial derivatives of the final coordinate X_k with respect to the corresponding initial coordinates $\{x_i\}$.

The mth power moment of the final variable X_k,

$$\mu_m=\langle X_k^m\rangle\equiv\int\int(X_k)^mF(\mathbf{X})d\mathbf{X} \tag{5}$$

can be calculated analytically if the initial PDF, $f(\mathbf{x})$ and the transfer map, $\mathcal{M}$ are known

$$\begin{aligned}\langle X_k^m\rangle&=\int\int(X_k)^mF(\mathbf{X})d\mathbf{X}\\&=\int\int(\mathcal{M}_k\circ\mathbf{x})^mf(\mathbf{x})d\mathbf{x}\\&=\int\int\left(\sum_{\{i_s\},\Sigma i_s\leqslant N}\mathcal{M}_{k,\{i_s\}}x_1^{i_1}\cdots x_6^{i_6}\right)^mf(\mathbf{x})d\mathbf{x}\\&=\sum_{\{j_s\},\Sigma j_s\leqslant mN}{}^mC_{k,\{j_s\}}\int\int x_1^{j_1}\cdots x_6^{j_6}f(\mathbf{x})d\mathbf{x}\\&=\sum_{\{j_s\},\Sigma j_s\leqslant mN}{}^mC_{k,\{j_s\}}\langle x_1^{j_1}x_2^{j_2}\rangle\langle x_3^{j_3}x_4^{j_4}\rangle\langle x_5^{j_5}x_6^{j_6}\rangle,\end{aligned} \tag{6}$$

where $\langle x_r^{j_r}x_t^{j_t}\rangle$ are the moments of the corresponding initial distributions f_{rt} and the coefficients ${}^mC_{k,\{j_s\}}$ are the products of m elements of the vector $\mathcal{M}_k$. The transition from the final variables $\mathbf{X}$ to the initial variables $\mathbf{x}$ in the second line of Eq. (6) is possible because the transfer map $\mathcal{M}$ is symplectic. In the last line of Eq. (6) we assumed the initial PDF $f(\mathbf{x})$ is given by Eq. (2).

One can analytically calculate any moment of the final distribution, $\langle X_1^{m_1}X_2^{m_2}\cdots X_6^{m_6}\rangle$ to arbitrary order N of the transfer map in a way similar to that of Eq. (6).

In an important particular case of the normal initial PDF [Eq. (3)], all the moments $\mu_{m,n}=\langle x_r^mx_t^n\rangle$ of the order $(m+n)$ can be expressed in terms of the second moments, $\langle x_r^2\rangle$, $\langle x_t^2\rangle$, and $\langle x_rx_t\rangle$ only. For numerical calculations of high-order moments $\mu_{m,n}$ of the bivariate normal distribution, it is convenient to use the following general formula:

$$\mu_{m,n}=\langle x_rx_t\rangle^n\langle x_r^2\rangle^{[(m-n)/2]}\sum_{j=0}^{q}\binom{n}{2j}\left[\frac{\langle x_r^2\rangle\langle x_t^2\rangle}{\langle x_rx_t\rangle^2}-1\right]^j\times[(m+n-2j-1)\,!!][(2j-1)\,!!], \tag{7}$$

if $(m+n)$ is even and $\mu_{m,n}=0$, if $(m+n)$ is odd. Here $m\geqslant n$, $(2j-1)!!\equiv1\times3\times5\times\cdots\times(2j-1)$ and $(-1)!!\equiv1$. The upper limit in the sum $q=n/2$ and $q=(n-1)/2$ for even and odd values of n, respectively.

For applications, most useful moments of the final distribution are the variances $\langle X_k^2\rangle_{k=1,3}$, which give the rms size of the beam, and the fourth moments $\langle X^4\rangle$, which indicate the weight of the tails of the distribution (beam halo). For example, if $Q_4=\langle X^4\rangle/\langle X^2\rangle^2>3$, the distribution has longer tails than the normal distribution, and if $Q_4<3$, the tails of the distribution die off more quickly than those of a Gaussian. For a description of the beam halo, there are also more complex combinations of the second and the fourth moments suggested [22], which relay on kinematic invariants and characterize "compactness" of the beam distribution in the two-dimensional (2D) phase space.

III. BEAM SHAPING USING MOMENTS

A. On the classical problem of moments

Let $x\in\mathbb{R}$ be a random variable with an (absolutely continuous) distribution function $\sigma(x)$ and a probability density function (PDF) $f(x)$. The real numbers

$$\mu_m\equiv\langle x^m\rangle=\int_{-\infty}^{\infty}x^md\sigma(x),\quad m=0,1,2,... \tag{8}$$

are the (power) moments of the distribution $\sigma(x)$. If $f(x)$ is symmetric, all its odd-order moments vanish. Let us summarize some notions and results of the classical theory of moments [23–25].

The *Hamburger moment problem* is formulated in the following way: given a set of real numbers $\{\mu_0,\mu_1,\mu_2,\ldots\}$, find all distributions $\sigma(x)$ such that

$$\int_{-\infty}^{\infty}x^md\sigma(x)=\mu_m,\quad m=0,1,2,\ldots\,. \tag{9}$$

The Hamburger moment problem is solvable if the Hankel matrix $(\mu_{m+n})_{m,n=0}^{\infty}\geqslant0$. In this case it can have a unique solution (a *determinate problem*) or an infinite number of solutions (an *indeterminate problem*).

Note that if $\sigma(x)\equiv$const for $x<0$ ($f(x)\equiv0$ for $x<0$), we have the Stieltjes moment problem and if $\sigma(x)\equiv$const for $x\notin[a,b]$ ($f(x)\equiv0$ for $x\notin[a,b]$), we deal with the Hausdorff finite interval problem. A solvable one-dimensional Hausdorff problem is always determinate.

In order that a Hamburger moment problem [Eq. (9)] shall have a solution, it is necessary that [25]

$$\Delta_n=\det(\mu_{i+j})_{i,j=0}^{n}\geqslant0,\quad n=0,1,2,\ldots\,. \tag{10}$$

The problem has an infinite number of solutions if and only if

TABLE I. Moments and moment-generating functions of normal, uniform, and parabolic distributions.

	$f(x)$	μ_{2m}	$M_x(s)$
Normal $a=\sigma$	$\frac{1}{a\sqrt{2\pi}}\exp\left[-\frac{x^2}{2a^2}\right]$	$(2m-1)!!a^{2m}$	$\exp\left[\frac{(as)^2}{2}\right]$
Uniform $-a\leqslant x\leqslant a$	$\frac{1}{2a}$	$\frac{a^{2m}}{2m+1}$	$\frac{\sinh as}{as}$
Parabolic $-a\leqslant x\leqslant a$	$\frac{3(a^2-x^2)}{4a^3}$	$\frac{3a^{2m}}{(2m+1)(2m+3)}$	$3\left[\frac{\cosh as}{(as)^2}-\frac{\sinh as}{(as)^3}\right]$

$$\Delta_n = \det(\mu_{i+j})_{i,j=0}^n > 0, \quad n=0,1,2,\ldots . \tag{11}$$

The moment problem [Eq. (9)] is determinate if and only if

$$\Delta_0 > 0, \ldots, \Delta_k > 0, \quad \Delta_{k+1} = \Delta_{k+2} = \cdots = 0. \tag{12}$$

The set of solutions of an indeterminate problem is in a one-to-one correspondence with a certain subset of the class of Nevanlinna functions [23].

A sufficient condition for the Hamburger moment problem to be determinate is that (*Carleman's criterion*) [23,25,29,30]

$$\sum_{m=1}^{\infty} (\mu_{2m})^{-1/2m} = \infty. \tag{13}$$

A corollary of the Carleman criterion [24,25,31] states that if the Hamburger moment problem has a solution, where $f(x) \geqslant 0$ and

$$\int_{-\infty}^{\infty} e^{\delta|x|}[f(x)]^q dx < \infty \tag{14}$$

for some $q\geqslant 1$ and $\delta>0$, then the problem is determinate, i.e., it has only one solution. As it follows from Krein's theorem [24], if

$$\int_{-\infty}^{\infty} \frac{\ln f(x)}{1+x^2} dx > -\infty, \tag{15}$$

the Hamburger moment problem [Eq. (9)] has an infinite number of solutions.

For example, the PDF

$$f_\alpha(x;\gamma) = \frac{\alpha\gamma^{1/\alpha}}{2\Gamma\left(\frac{1}{\alpha}\right)}\exp(-\gamma|x|^\alpha), \quad \alpha,\gamma > 0, \tag{16}$$

where $\Gamma(z)$ is the Euler Γ function, has an infinite number of moments for any positive α. However, as it stems from the Carleman criterion [Eq. (13)], the corresponding Hamburger moment problem has a unique solution [Eq. (16)] only if $\alpha > 1$. In particular, the normal PDF with $\alpha=2$ and $\gamma=1/2\sigma^2$. If $\alpha\leqslant 1$, this problem has an infinite number of solutions described by the Nevanlinna formula [23]. Other examples of moment sets $\{\mu_m\}_{m=0}^{\infty}$, which generate indeterminate moment problems, are provided in [23,24].

A *truncated* Hamburger moment problem [23] —a moment problem with a finite set of given numbers (i.e., $\{\mu_m\}_{m=0}^{2\nu}$, $\nu=0,1,2,\ldots$)—is solvable if the Hankel matrix $\Gamma_\nu = (\mu_{m+n})_{m,n=0}^{\nu} > 0$ [26–28]. In the degenerate case of a singular Hankel matrix Γ_ν the problem of moments (under some special conditions established in [26–28]) has a unique solution described in [26,27].

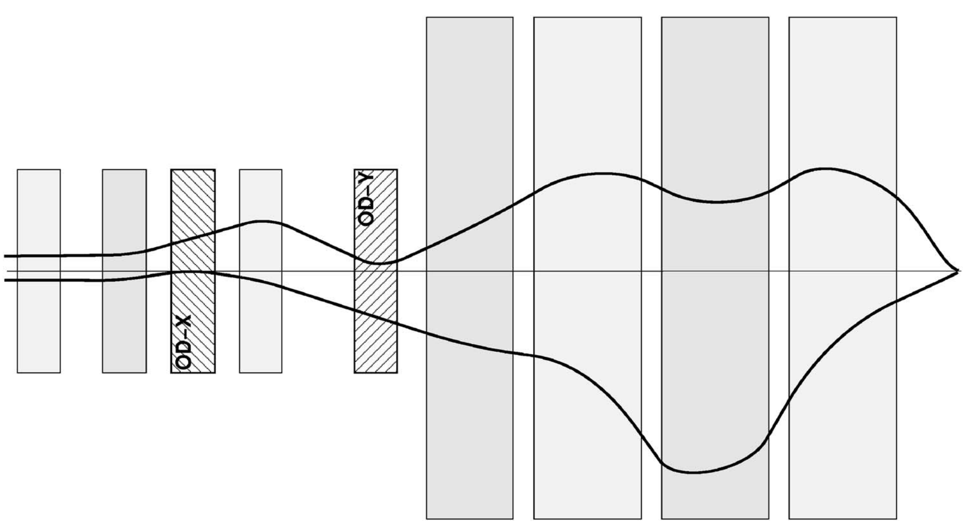

FIG. 1. Layout of the HEDgeHOB final focus system and the beam envelopes (not in scale). Nonlinear-shaping optical elements (combined octupole and duodecapole magnets, $L=1$ m, $R=6$ cm), OD-X and OD-Y are shown as hatched bars.

If in a neighborhood of the point $s=0$ there exists the *moment-generating function* (MGF)

$$M_x(s) \equiv \langle e^{sx} \rangle = \int_{-\infty}^{\infty} e^{sx} f(x) dx = \sum_{m=0}^{\infty} \mu_m \frac{s^m}{m!}, \qquad (17)$$

then the PDF, $f(x)$, and its moments can be expressed through the MGF, $M_x(s)$, uniquely,

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-isx} M_x(is) ds,$$

$$\mu_m = \left. \frac{d^m}{ds^m} M_x(s) \right|_{s=0}. \qquad (18)$$

Note that, for example, for the PDF [Eq. (16)] with $\alpha \leqslant 1$, the MGF exists only at the point $s=0$ (the zero moment) and cannot be prolongated analytically to a vicinity of this point. Therefore the problem in this case is indeterminate.

B. Fitting the moments of the final distribution

In the material given below we deal with *a priori* solvable moment problems only. The remaining question, therefore, is the uniqueness of the reconstruction of a (one-dimensional) PDF by its power moments, $\{\mu_m\}_{m=0}^{\infty}$.

The conditions of uniqueness of the solution given in Sec. III A hold for the probability distributions of practical interest. For example, moments and moment-generating functions of normal, uniform, and parabolic PDFs are shown in Table I. The latter two distributions correspond to the determinate Hausdorff problems, like any other so-called bounded PDFs, which are always uniquely determined by their infinite set of moments. Due to the Carleman criterion, the normal PDF is determined by its moments in the unique way as well, as it has been discussed above.

We presume that if the series of Eq. (17) converges fast enough, it should be possible to approach a desired PDF by controlling a finite (small) number of nonzero first moments of the target PDF, $\{\mu_m\}_{m=0}^{n}$. This presumption is justified by the numerical results presented in Sec. IV.

In Sec. II we have shown how one can calculate an arbitrary moment $\langle X_k^m \rangle$ analytically, if the moments of the initial distribution and the transfer map of the system are known. In order to calculate the mth moment of the final variable using the Nth-order transfer map, all the moments of the initial distribution up to the order mN have to be known. These moments can be either calculated for a certain analytic initial distribution or taken from measurements. If an optical system contains nonlinear elements (e.g., high-order multipoles such as octupoles and duodecapoles), then it is possible to control the moments of the final distribution by adjusting the fields in the corresponding magnets. In turn, by fitting a set of moments of the final PDF, $F_k(X_k)$, one can approach a desired distribution of any variable X_k. This will also automatically account for any coupling between transverse or longitudinal phase planes and other effects, such as fringe fields.

The number of final moments to be fitted, sufficient to approach a goal distribution, depends, in general, on particular initial and final distributions and on the number of degrees of freedom of an optical system, i.e., the number and location of nonlinear elements. Usually, good results can already be obtained by fitting the second and the fourth moments, whereas including into the fit some higher-order moments (sixth, eighth, tenth, and twelvth) makes only minor improvements. The quality of the shaping also depends on the beam emittance and desired width of the final distribution: the smaller the beam emittance and the larger the spot size, the better one can approach the desired distribution shape. In the following section some examples of calculation using the developed shaping technique for a practical application are presented.

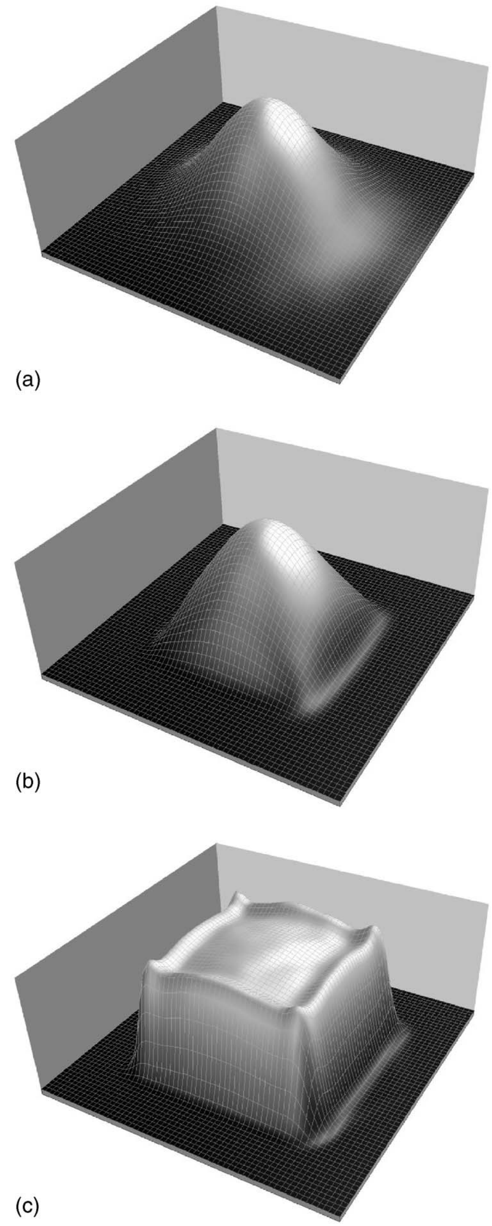

FIG. 2. Transverse distribution of the beam intensity after the system: (a) Gaussian distribution (nonlinear elements were switched off), (b) parabolic distribution, and (c) uniform distribution. The parabolic (b) and uniform (c) distributions have the same width; distributions (a) and (c) have equal dispersions.

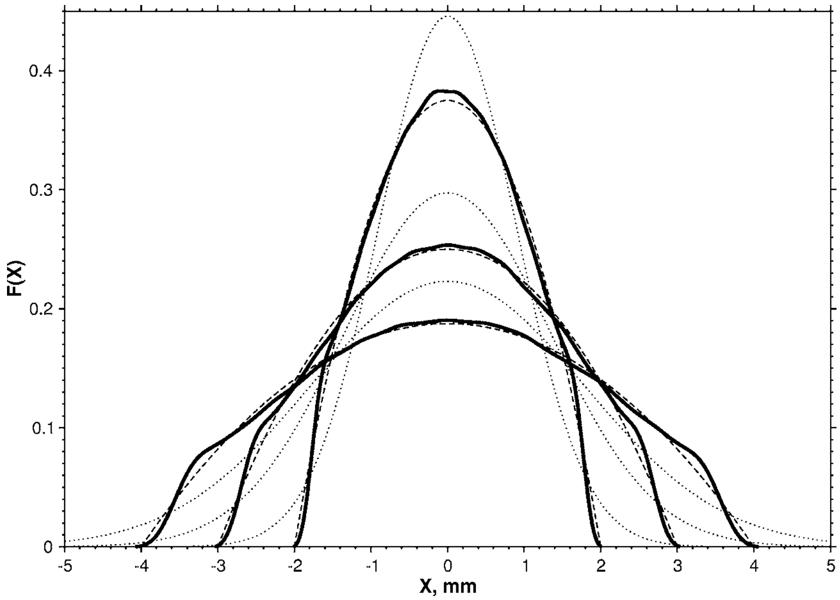

FIG. 3. Shaping a Gaussian beam to parabolic distributions of different width (a=2, 3, and 4 mm): Solid lines, result of shaping (fifth-order transfer map, the nonzero power moments up to eighth-order were fitted); dashed lines, ideal parabolic distributions; and dotted lines, Gaussian distributions with the corresponding dispersion.

IV. CALCULATION EXAMPLES

In order to demonstrate usefulness of the suggested theoretical approach, a number of numerical calculations on beam shaping using the power moments has been carried out. For these calculations, one of the current designs of the transport and final focus system for the proposed HEDgeHOB (high energy density matter generated by heavy ion beams) collaboration experiments [14] at FAIR (Facility for Antiproton and Ion Research) in Darmstadt, Germany has been chosen. The layout of the optical system is shown in Fig. 1.

Two nonlinear elements (combined octupole and duodecapole magnets) have been introduced into the final focus system. To minimize the coupling between the transverse phase planes, the nonlinear elements are placed at the positions where the beam envelop is large in one plane and small in the other (see Fig. 1). Realistic initial beam parameters and Gaussian initial phase-space distribution [Eqs. (2) and (3)] have been assumed. The normalized rms beam emittance ($\epsilon_x^{\text{rms}} \times \epsilon_y^{\text{rms}}$) of (6.3×2.0) mm mrad corresponds to the design value of the SIS-100 heavy ion synchrotron at FAIR.

Beam physics code COSY INFINITY version 8.1 [32] has been employed in the calculations. Since this code is based on differential algebraic methods, it is able to compute an arbitrary-order transfer map of an optical system. The code also provides a powerful work environment with the high-level programing language, COSY, and elaborate optimization algorithms. The procedures for calculating initial and final distribution moments have been written in the COSY language. Special efforts have been made to optimize the algorithm and procedures, which calculate high-order final moments, since they are called many times during the fitting cycle.

Two series of calculations have been carried out: the beam with initially Gaussian distribution has been shaped to obtain the parabolic and uniform (see Table I) transverse distributions in the focal spot behind the system. In both cases, the calculations were performed for different final distribution widths (focal spot size) of a=2, 3, and 4 mm.

During the calculations, x- and y-plane moments, $\{\langle X_1^m\rangle\}_{m=2}^n$ and $\{\langle X_3^m\rangle\}_{m=2}^n$, were fitted to the desired values, simultaneously, in order to obtain equal final distributions $F_1(X_1)$ and $F_3(X_3)$ after the system ("anastigmatic shaping"). A weighted sum of relative residuals,

$$G = \sum_{m=2}^{n} w_m \left(\frac{Q_m - Q_m^{\text{th}}}{\frac{1}{2}(Q_m + Q_m^{\text{th}})} \right)^2, \quad (19)$$

where $Q_2=\langle X_k^2\rangle$, $Q_m=\langle X_k^m\rangle / \langle X_k^2\rangle^{m/2}$, and Q_m^{th} are the corresponding theoretical values for a certain final distribution (see Table I) has been minimized.

The transfer map of the system has been calculated to the fifth order, and the sets of final moments from n=2 to n=12 were fitted. Although the coupling between the phase planes in this system is almost negligible, it has been taken into account while calculating the final moments.

The minimum of the goal function [Eq. (19)] was obtained by varying the octupole and duodecapole field components of the two nonlinear elements, as well as the field intensities in the last four quadrupoles (Fig. 1). After the fitting, the transverse distribution in the focal spot was determined by performing a Monte Carlo particle tracking. Typical examples of the obtained 2D transverse distributions are shown in Fig. 2.

In Fig. 2(a) the results of the calculation with all nonlinear field components switched off are presented. The shape of the initial (Gaussian) distribution, therefore, remains unchanged, while only the focal spot size (x and y dispersion of the distribution) varies after the beam passes through the final focus system. The results of shaping the beam to parabolic and uniform distributions of the same width are shown in Figs. 2(b) and 2(c), respectively. Remarkable here are the strong suppression of the distribution tails (beam halo) and the characteristic "rectangular" pattern of the transverse distributions, resulting from the twofold symmetry of the multipole magnetic fields.

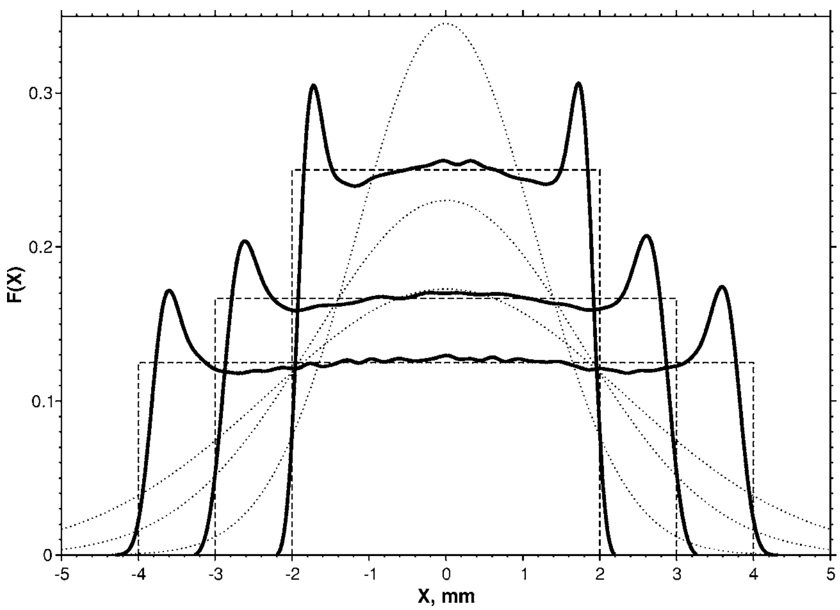

FIG. 4. Shaping a Gaussian beam to uniform distributions of different width (see caption of Fig. 3).

A more detailed view on the calculation results is given in Figs. 3 and 4, where the marginal beam PDFs in the focal spot, $F_1(X_1)$ [the distributions $F_3(X_3)$ look similar, see Fig. 2] are shown. The results of shaping calculations for the parabolic distribution are shown in Fig. 3 and, for the uniform distribution, in Fig. 4. In both cases, different distribution widths (focal spot size) of $a=2$, 3, and 4 mm were chosen. In the same plots, the goal distributions (dashed lines) and the corresponding Gaussian distributions (dotted lines) are shown for comparison.

From the presented calculation examples one can see that, even for such a simple system containing only two nonlinear elements, it is possible to approach various transverse beam intensity distributions with a good accuracy. The small "knees" on the slopes of the obtained parabolic distributions (Fig. 3) are caused by the symmetry issues of the optical system. Although the spikes near the edges of the uniform PDFs (Fig. 4) cannot be fully eliminated, they are less pronounced if one looks at a distribution near the beam axis (Fig. 2) rather than at the marginal PDF shown in Fig. 4. The weight of these peaks depends on the beam emittance and the desired width of the distribution: better results can be obtained for a beam-expander system than for a final focus system.

It is to be noted that the suggested shaping method and the corresponding computer codes can be applied to any initial or final PDFs and to an arbitrary optical system. The applications of the developed beam shaping approach to the problem of controlling beam losses in high-energy high-intensity accelerators are foreseen.

V. SUMMARY

A method for beam shaping is suggested. This method is based on the explicit calculation of power moments of the final phase-space distribution uniquely determined by its infinite set of moments and the minimization of the deviation of a truncated final moment set from the prescribed values of the moments. This approach allows one to obtain a desired beam intensity PDF without making special assumptions on the optical system characteristics. The presented calculation examples for the HEDgeHOB final focus system demonstrate that this statistical approach to the beam shaping works quite well and is reliable.

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