FUNDAMENTAL ASPECTS OF THE MOMENT PROBLEM FOR A PARTICLE DENSITY EVOLVING UNDER NON-LINEAR FORCES

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Abstract

A statistical description (moments) of a beam can be (and has already been) foreseen to study its evolution when the force is not linear. We analyse why this approach leads to severe difficulties, and we present fundamental aspects, based on orthogonal polynomials [1]. A key point is the calculation of high order unknown moments (either for tracking or for particle localization). They can be estimated by extrapolation of recurrence relations. The analysis is generalized to a 2D phase space, and shows the limits of such techniques, already difficult in 2D, for accelerator physics in 6D. Finally, we show what kind of maximum information can be obtained from a finite number of moments like a good estimate of the particle localization and density.

1 INTRODUCTION

High power accelerators of several MW have strongly motivated the study of halo under non-linear space charge, by the mean of several kinds of codes (PCM, PIC, PPI). The accuracy needs (up to 10^{-9}) request a very large number of particles for the PPI model. It seems to be encouraging to study only the evolution of the statistical parameters of the beam density. The moments of a 1D or 2D density ω,defined over Ω, are respectively given by :

$$\mu_n = \int_\Omega x^n \omega(x) dx \text{ and } \mu_{nm} = \int_\Omega x^n \dot{x}^m \omega(x,\dot{x}) dx d\dot{x} \quad (1)$$

We work with derivatives versus time (dot symbols). We consider in the whole paper, as an illustration, the evolution of particles whose initial density (in the $(x,\dot{x})$ phase space) is uniform in the unity disk. We suppose also that the force is stationary and equal to $\alpha x+\beta x^p$ (p>1). One observes, at different times, filamentation up to equilibrium (Fig. 1).

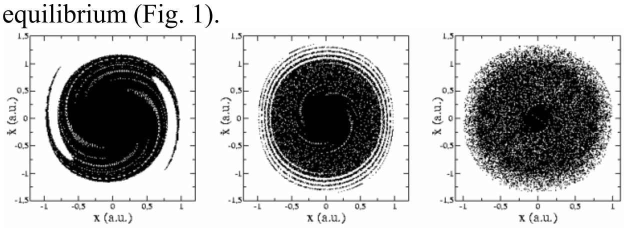

Figure 1: evolution with a non-linear force

In such case, the evolution of the moments is given by:

$$\frac{dx^n \dot{x}^m}{dt} = n x^{n-1} \dot{x}^{m+1} + m\left(\alpha x^{n+1} \dot{x}^{m-1} + \beta x^{n+p} \dot{x}^{m-1}\right) \quad (2)$$

$$\dot{\mu}_{nm} = n\mu_{n-1,m+1} + m\left(\alpha\mu_{n+1,m-1} + \beta\mu_{n+p,m-1}\right) \quad (3)$$

As only a finite number of moments are known, the estimation of high order moments ("HOMs") is necessary. This example shows the difficulty, even in 2D, and the fundamental questions we will investigate, in terms of statistical moments: Where are the particles located? What is the information contained in moments? What is the equilibrium density? Is it possible to calculate high order moments?

2 APPROACH WITH MACROPARTICLES

In the 2D case, we can always find a set macroparticles, defined by their position $(x_i, \dot{x}_i)$ and their weight λ_i, whose moments are those of the original density, up to degree N. They are not unique. The known moments of order n+m≤N can be written:

$$\mu_{nm} = \sum_{i=1}^{N} \lambda_i x_i^n \dot{x}_i^m \quad (4)$$

Starting from the uniform density, we can study for example the evolution of the RMS emittance, related Fig 2. It is easy to show that macroparticle tracking, with constant weights, is equivalent to extrapolate HOMs by using the above formula with n+m>N.

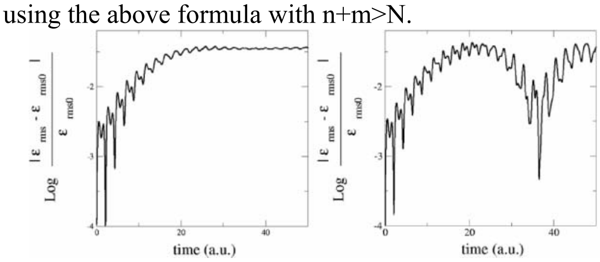

Figure 2: evolution of the relative emittance of the disk uniform density (log scale). Left: tracking of 32000 particles. Right: tracking of 64 macroparticles.

Fig 2 shows a very good accuracy for the transient phase, but the long term evolution does not reproduce correctly the equilibrium. This is due to the quasi-periodicity of the set of macroparticles. This first "naïve"analysis shows that HOMs must be accurately estimated, and not roughly or, worse, be set equal to zero (truncation of the evolution equation) in some publications.

3 A RIGOUROUS APPROACH

The basic idea is to analyse the problem in 1D case, by working with orthogonal polynomials, which provide a deeper description of the problem. In fact, the extrapolation of HOMs must keep basic properties of orthogonal polynomials, like zero interlacing. Adding these properties will lead to a better understanding and an increase of accuracy. Some results given below are classical, some of them are new.

3.1 Moments and orthogonal polynomials in 1D

Let us consider the moments μ_n ($n\leq 2N$) of a 1D density ω. They can be written [2] rigorously by the quadrature relation:

$$\mu_n = \int_\Omega x^n \omega(x)dx = \sum_{i=1}^{N} \lambda_i x_i^n \qquad (5)$$

x_i are the zeroes of P_N the N^{th} degree orthogonal polynomial associated to ω and λ_i are the Christoffel coefficients. If p_{ij} is the coefficient of degree i of P_j, the two NxN P and Q matrixes defined by:

$$Q = \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_N \\ \mu_1 & \mu_2 & \cdots & \mu_{N+1} \\ \cdots & \cdots & \cdots & \cdots \\ \mu_N & \mu_{N+1} & \cdots & \mu_{2N} \end{bmatrix} \qquad (6)$$

$$\mathrm{P} = \begin{bmatrix} p_{00} & 0 & \cdots & 0 \\ p_{10} & p_{11} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ p_{N0} & p_{n1} & \cdots & p_{NN} \end{bmatrix}$$

fulfil the relation:

$$PQ\widetilde{P} = I \qquad (7)$$

where ~ is the transposition and I the identity matrix.

So, the P matrix is easily obtained by calculating the inverse matrix of the Cholesky decomposition of Q. These polynomials are normalized (their quadratic integral weighted by ω is 1). Moments and polynomials are related in a simple way, which permits HOMs calculation from an estimation of the high order polynomials ("HOPs"):

$$\sum_{i=0}^{m} p_{mi}\mu_{n+i} = 0 \text{ for } m > n \qquad (8)$$

Three successive orthogonal polynomials satisfy to a recurrence relation (written here for ω even):

$$P_{n+1}(x) = b_{n+1}xP_n(x) + c_{n+1}P_{n-1}(x) \qquad (9$$

This implies that the zeroes of successive polynomials are interlaced in the convex hull of Ω (Figure 3).

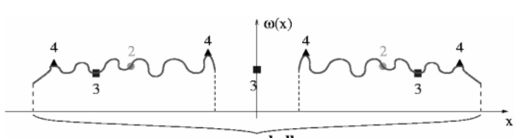

Figure 3: zeroes of successive polynomials

The Stieljes transform of ω is defined below and can be developed in series, showing how moments describe, the global outside description of the density.

$$F(x) = \int_\Omega \frac{\omega(\xi)d\xi}{x-\xi} = \sum_{j=0}^{+\infty} \frac{\mu_j}{x^{j+1}} \qquad (9)$$

The [N-1,N] Pade approximant to F, who (by definition) has the same development in series up to ordre N, is related [3] to P_N (T_N is a non important polynom) and can also be writen:

$$F_{[N-1,N]}(x) = \frac{T_N}{P_N}(x) = \sum_{j=0}^{2N} \frac{\mu_j}{x^{j+1}} + \frac{\hat{\mu}_{2N+1}}{x^{2N+1}} + \cdots \qquad (10)$$

The high order terms of $F_{[N-1,N]}$ are the HOMs obtained by using the quadrature relation (5) for n>2N ("extrapolation"). Its poles are the zeroes of P_N.

Conclusion: a finite set of moments gives only information about the convex hull of Ω. Modelization must be made in terms of poles. The extrapolation of HOMs will be done by extrapolating HOPs. This philosophy is used in paragraph 3.2.

3.2 1-D High Order Moments. Support of ω

We use recurrence relation(9) to estimate HOPs. A natural question is the convergence properties of b_n and c_n. We give (Fig 4 and 5), two examples of ω and b_n. We have either convergence of the sequence or convergence of sub-sequences, corresponding to the number of lobes of ω.

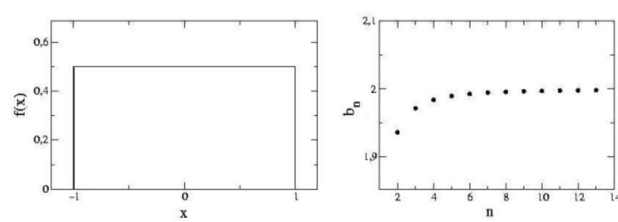

Figure 4: uniform density and b_n coefficients

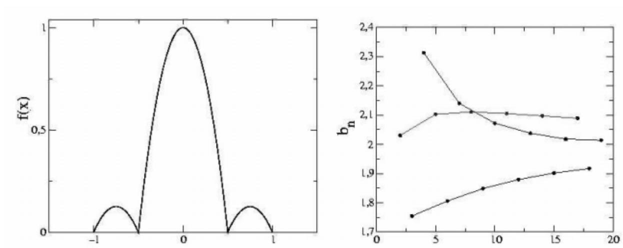

Figure 5: 3-lobes density and b_n sequence. Three converging sub-sequences are drawn, corresponding to the 3 lobes of the density. This kind of figure occurs for x-profile in case of filamentation.

We have seen that extrapolation of quadrature formulas did not give good results. In fact, it is equivalent to take c_n

equal to zero for n>N. From examples given above, we see that it is not correct and does not preserve the zeroes interlacing. A better solution is to look at the number of converging sub-sequences and to estimate their limits. This gives the convex hull of ω. For example, if we consider a “1-lobe” density, (Fig 4), and take the last known coefficients as the limit, (9) becomes:

$$P_{n+1}(x) = bxP_n(x) + cP_{n-1}(x) \quad (n > N) \qquad (11)$$

Let’s construct functions having poles, in the convex hull:

$$Q_{n+1}(x) = \frac{P_{n+1}(x)}{P_n(x)} = bx + \frac{c}{Q_n(x)} \qquad (12)$$

This sequence converges only out of the convex hull. The limit is solution of a second degree equation, whose discriminant (depending on x) is negative out of the convex hull. This can be written:

$$|x| < 2\sqrt{\frac{-c}{b}} \qquad (13)$$

For the uniform density over [-1,1], by using moments up to the 8th order, the bound is found to be 1.0022 instead of 1. This kind of calculation has been made also in the case of several converging sub-sequences [1]. It is fundamental to estimate accurately the bounds, in order to be able to reconstruct the density profile.

3.3 Density Reconstruction

Once the support is well estimated, the density can be reconstructed by developing it on a Legendre basis (orthogonal polynomials of the uniform density on the support of ω). For example, suppose a density defined on [-a,a] and let us develop it on a classical Legendre basis:

$$\omega(x) = \sum_{j=0}^{n} \sigma_j P_j^L\left(\frac{x}{a}\right) \text{with}\ \sigma_{\mathrm{j}} = \sum_{k=0}^{j} p_{jk}^L \frac{\mu_k}{a^k} \qquad (14)$$

Figure 6 shows an example of reconstruction. The accurate estimate of a is mandatory to get the right shape of w and then to get the right HOMs (from formula 8).

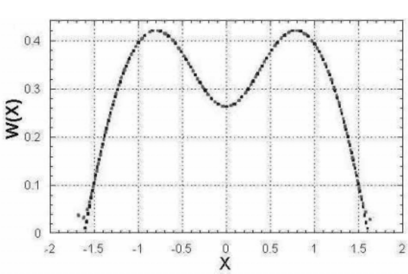

Figure 6: Example of a density reconstruction

3.3 2D case

We think in terms of poles and convexity. We consider the integral developed versus the nth order moments.

$$F(x,\dot{x}) = \int_\Omega \frac{\omega(\xi,\eta)d\xi d\eta}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} \equiv \sum_{n=0}^{+\infty} f_n(x,\dot{x}) \sum_{p=0}^{n} \mu_{p,n-p}$$

It is written in polar coordinates, versus $M_{\theta n}$ the nth moments of the projection of ω on the line whose azimuth is θ:

$$F(x,\dot{x}) = F_\vartheta(\rho) = \sum_{n=0}^{+\infty} \frac{M_{\theta n}}{\rho^{n+1}} \qquad (16)$$

For each value of θ we estimate the edge of the distribution by using the formalism of 3.2. Examples of the convex envelope are given figure 7 at different times.

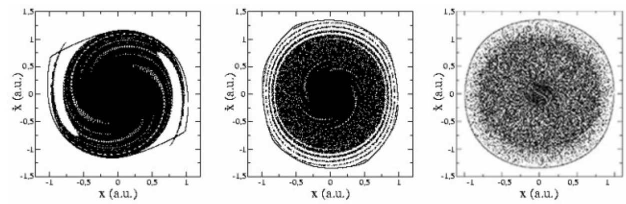

Figure 7: convex envelopes of 10^5 particles, obtained from the up 10th order 2D moments. Less than 10 particles are outside.

Finally, we have made some moment tracking using this formalism and supposing 1-lobe projected density (a 3 or more lobes should have been considered to consider really filamentation). We obtain now figure 8, which has to be compared to Figure 2, with a clear improvement even if we are limited to a small emittance increase.

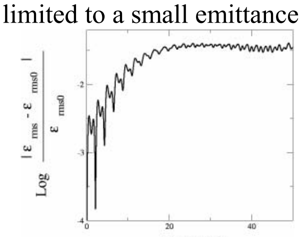

Figure 8: emittance increase by moment tracking.

4 CONCLUSION

We have shown how to get maximum information from the moments, but also fundamental limitations. It has to be considered in terms of poles and convexity (some information is definitely lost). Multi-lobe analysis has to be developed to make a good moment tracking in 2 dimensions. Higher dimensions have not been considered.

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