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THE MOMENT APPROACH TO CHARGED PARTICLE BEAM DYNAMICS*

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Summary

We have derived the hierarchy of moment equations that describes the dynamics of charged particle beams in linear accelerators and can truncate the hierarchy at any level either by discarding higher moments or by a cumulant expansion discarding only correlation functions. We have developed a procedure for relating the density expansion linearly to the moments to any order. The relation of space-charge fields to the density has been derived; and an accurate, systematic, and computationally convenient expansion of the resultant integrals has been developed.

Introduction

The dynamics of charged particle beams involves a large number of degrees of freedom; consequently, the solution of the equations of motion and the interpretation of solutions is quite difficult. The approximate reduction of the equations of motion to a finite system, in analogy with reduction of the equations for a solid body to Euler equations, would be very useful both for numerical computation and for intuitive interpretation. However, because a charged particle beam is not a perfect solid body, even in phase space, it is important to correct systematically the lowest order equations to any desired order.

How to derive moment equations to describe beam dynamics in three dimensions to any arbitrary order is shown in this paper. The truncation of these equations at any order is discussed, and how to compute space-charge forces in terms of the moments consistently to the same order is shown.

Basic Equations

For simplicity, let us consider nonrelativistic beams in which the space charge is well described by electrostatic forces. Also, we ignore the effects of walls and of particle collisions. None of these approximations are essential to our development, but are reasonably well satisfied for some low-energy proton linacs. Thus the equations we derive, besides being simple, are directly applicable to some machines. With these assumptions, the beam obeys the Vlasov equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} + \frac{1}{m} (\vec{F} + q\vec{E}) \cdot \frac{\partial f}{\partial \vec{v}} = 0 \quad , \tag{1}$$

where $f(\vec{x},\vec{v},t)$ is the distribution function in phase space, m is the mass of the particles, $\vec{F}(\vec{x},t)$ is the external force caused by the accelerating and focusing structure, and $\vec{E}$ is the space-charge electric field that satisfies

$$\vec{\nabla} \cdot \vec{E} = 4\pi q \int d\vec{v}\, f(\vec{x},\vec{v},t) \quad . \tag{2}$$

If we denote the total number of particles by N, then integrating Eq. (1) over $\vec{x}$ and $\vec{v}$ gives

$$\frac{dN}{dt} = 0 \quad , \tag{3}$$

where we ignore possible losses to the walls. If $g(\vec{x},\vec{v},t)$ is any function defined on phase space, let us define an average by

$$\langle g \rangle \equiv \frac{1}{N} \int d\vec{x} d\vec{v}\, g(\vec{x},\vec{v},t)\, f(\vec{x},\vec{v},t) \quad . \tag{4}$$

Note that $\langle g \rangle$ remains a function of time.

Multiplying Eq. (1) by x_i (the ith component of the spatial variable) and integrating over phase space, we find (see Appendix)

$$\frac{d\langle x_i \rangle}{dt} = \langle v_i \rangle \quad ; \tag{5}$$

that is, the center of mass moves at the average velocity. Multiplying Eq. (1) by v_i and integrating, we find

$$\frac{d\langle v_i \rangle}{dt} = \frac{1}{m} \langle F_i + qE_i \rangle \quad ; \tag{6}$$

that is, the average acceleration is the average of the forces over the mass.

Multiplying Eq. (1) by $x_i x_j$, $x_i v_j$, $v_i v_j$ and integrating we obtain, respectively,

$$\frac{d}{dt} \langle x_i x_j \rangle = \langle x_i v_j \rangle + \langle x_j v_i \rangle \quad , \tag{7}$$

$$\frac{d}{dt} \langle x_i v_j \rangle = \langle v_i v_j \rangle + \frac{1}{m} \langle x_i (F_j + qE_j) \rangle \quad , \text{and} \tag{8}$$

$$\frac{d}{dt} \langle v_i v_j \rangle = \frac{1}{m} \langle v_i (F_j + qE_j) \rangle + \frac{1}{m} \langle v_j (F_i + qE_i) \rangle \quad . \tag{9}$$

Let us make several comments about these equations. First, note that Eqs. (5)-(9) are exact and thus can be used directly to check particle simulation codes. Next, note that the forces depend on the spatial variables, and thus Eqs. (5)-(9) are not closed unless the forces are spatially linear. The assumption of linear forces gives the lowest significant truncation of the moment equations. Let us note that the second-order moments have a fairly direct physical interpretation. In the center of mass frame of reference, $\langle x^2 \rangle$ is the width of the phase space "ellipse," $\langle v^2 \rangle$ is its height, and $\langle xv \rangle$ is proportional to the tangent of the angle of the "ellipse" with respect to the axis. The description of the phase-space distribution in terms of ellipses is not exact, of course; in fact it corresponds exactly to the truncation of the moment equations at second moments, that is, to the approximation of linear forces. Finally, let us note that in the approximation of linear forces, it is easy to see that in the center of mass we have

$$\frac{d}{dt}\left(\langle x^2 \rangle \langle v_x^2 \rangle - \langle x v_x \rangle^2 \right) = 0 \quad ; \tag{10}$$

that is, emittances are preserved. Thus emittance growth can result only from nonlinear forces.

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The extension of the moment equations to arbitrary order proceeds as before and is perfectly straightforward. Let us write out the third moment equations explicitly:

$$\frac{d}{dt}\langle x_i x_j x_k\rangle = \langle v_i x_j x_k\rangle + \langle x_i v_j x_k\rangle + \langle x_i x_j v_k\rangle \quad , \tag{11}$$

$$\frac{d}{dt}\langle x_i x_j v_k\rangle = \langle v_i x_j v_k\rangle + \langle x_i v_j v_k\rangle + \frac{1}{m}\langle x_i x_j (F_k + qE_k)\rangle \quad , \tag{12}$$

$$\frac{d}{dt}\langle x_i v_j v_k\rangle = \langle v_i v_j v_k\rangle + \frac{1}{m}\Big\{\langle x_i x_k (F_j + qE_j)\rangle + \langle x_i v_j (F_k + qE_k)\rangle\Big\} \text{ , and} \tag{13}$$

$$\frac{d}{dt}\langle v_i v_j v_k\rangle = \frac{1}{m}\Big\{\langle v_i v_j (F_k + qE_k)\rangle + \langle v_i v_k (F_j + qE_j)\rangle + \langle v_j v_k (F_i + qE_i)\rangle\Big\} \quad . \tag{14}$$

Once again, these equations are not closed unless all forces are linear.

Let us make two comments about the moment equations at any order. First we observe that the forces generally will have an expansion in spatial variables that does not truncate at finite order. Thus the equations for the nth moments involve all higher moments. If we truncate the spatial expansion of the forces at mth order, the nth moment equations still involve (n + m)th moments so that a truncation of the moments is still required; truncation of the forces produces smooth forces, and thus eliminates the more obvious "collisional" effects that can arise in particle codes. Secondly, let us observe that the number of equations is surprisingly small: through fourth moments there are only 209 first-order equations (923 through sixth moments), which is roughly the same number as the equations of motion for 35 particles.

Before the moment equations can be useful, we must discuss two problems: truncation of the equations and calculation of the forces.

There is no unique truncation procedure for closing the moment equations, of course. The simplest procedure is to ignore, that is, set to zero, all moments higher than the desired order. In general there is no reason to believe that this procedure should be very accurate. A better-motivated procedure is to include the relevant higher order moments but to ignore higher order correlations, that is, to approximate the higher order moments as products of lower order moments. Again, there is no unique prescription, but a reasonable truncation is illustrated by the approximation

$$\langle x_i x_j x_k\rangle \simeq \langle x_i\rangle\langle x_j x_k\rangle + \langle x_j\rangle\langle x_i x_k\rangle + \langle x_k\rangle\langle x_i x_j\rangle \quad . \tag{15}$$

We assume that the external force, $\vec{F}(\vec{x},t)$, is known once the accelerator is specified. The greater difficulty lies in the calculation of the space-charge force. If we define

$$\rho(\vec{x},t) \equiv \int d\vec{v}\, f(\vec{x},\vec{v},t) \quad , \tag{16}$$

and

$$\vec{E} = -\vec{\nabla}\phi \quad , \tag{17}$$

then the solution of Eq. (2) can be written

$$\phi(x,t) = \int \frac{d\vec{x}'\,\rho(\vec{x}',t)}{|\vec{x} - \vec{x}'|} \quad , \tag{18}$$

where, once again, we ignore the influence of walls.

If we define

$$\tilde{\vec{x}} \equiv \vec{x} - \langle\vec{x}\rangle \quad , \tag{19}$$

then it is reasonable to expand Eq. (18) as

$$\phi(\tilde{\vec{x}},t) = A_i(t)\tilde{x}_i + B_{ij}(t)\tilde{x}_i\tilde{x}_j + C_{ijk}(t)\tilde{x}_i\tilde{x}_j\tilde{x}_k + \ldots \quad , \tag{20}$$

where we have used the summation convention, and where

$$A_i(t) = \int \frac{d\tilde{\vec{x}}'\,\tilde{x}_i'\,\rho(\tilde{x}',t)}{\tilde{r}'^3} \quad , \tag{21}$$

$$B_{ij}(t) = \frac{1}{2}\int \frac{d\tilde{\vec{x}}'}{\tilde{r}'^3}\left(\tilde{x}_i' \frac{\partial\rho}{\partial\tilde{x}_j'} + \tilde{x}_j' \frac{\partial\rho}{\partial\tilde{x}_i'}\right) \text{ , and} \tag{22}$$

$$C_{ijk} = \frac{1}{6}\int \frac{d\tilde{\vec{x}}'}{\tilde{r}'^3}\left(\tilde{x}_i' \frac{\partial^2\rho}{\partial\tilde{x}_j'\partial\tilde{x}_\ell'} + \text{symmetric combinations}\right) \quad . \tag{23}$$

This expansion clearly can be carried to any order. We must now relate the charge density, $\rho(\vec{x},t)$, to the moments; we will then have the right-hand sides of the moment equations specified entirely in terms of external forces and moments.

There is no unique relation between ρ and the spatial moments; we must assume some model for ρ. We assume

$$\rho(\tilde{\vec{x}},t) = \exp\left[-F_{ij}(t)\tilde{x}_i\tilde{x}_j\right]\Big\{\alpha + \exp\left(-\beta_1\tilde{r}^2\right)\left[\epsilon_i^{(t)}\tilde{x}_i + \gamma_{ijk}^{(t)}\tilde{x}_i\tilde{x}_j\tilde{x}_k + \ldots\right] + \exp\left(-\beta_2\tilde{r}^2\right)\left[K_{ij}^{(t)}\tilde{x}_i\tilde{x}_j + \lambda_{ijk\ell}^{(t)}\tilde{x}_i\tilde{x}_j\tilde{x}_k\tilde{x}_\ell + \ldots\right]\Big\} \quad , \tag{24}$$

where β_1 and β_2 are constants. Roughly speaking, we put the second-moment information into F_{ij} and insert the additional Gaussians to ensure nonnegative densities. If we require that the higher order terms, terms following α in Eq. (24), produce no change in the first and second moments, then the $F_{ij}(t)$ are simply related to the second moments, and the $\epsilon_i(t)$, $\gamma_{ijk}(t)$, $K_{ij}(t)$, $\lambda_{ijk\ell}(t)$, ... are linearly related to the higher moments.

We have now completely specified the equations to be solved. However, we still have three-dimensional integrals, as in Eq. (21)-(23), to compute. A typical integral that enters is

$$I = \int \frac{d\vec{x}}{r^3} \exp\left\{-\lambda_1 x_1^2 - \lambda_2 x_2^2 - \lambda_3 x_3^2\right\} x_1^m x_2^n x_3^p \quad , \tag{25}$$

where $\lambda_i(t)$ are constants in space, and m,n,p are integers (possibly zero). A useful technique for evaluating this integral is to "expand about the sphere"; that is, let

$$\overline{\lambda} = \frac{1}{2}\left\{\max(\lambda_i) + \min(\lambda_i)\right\} \quad , \tag{26}$$

and expand

$$I = \int \frac{d\vec{x}}{r^3} e^{-\overline{\lambda} r^2} x_1^m x_2^n x_3^p \Big[1 - (\lambda_1 - \overline{\lambda})x_1^2 - (\lambda_2 - \overline{\lambda})x_2^2$$

$$- (\lambda_3 - \overline{\lambda})x_3^2 + \ldots\Big] \quad . \tag{27}$$

Each integral in this expansion now can be done analytically, and the expansion can be carried out to any desired accuracy. Naturally, this expansion is most useful for bunches that are not too long. For very long bunches, we cannot justify the neglect of boundary conditions, and a different treatment must be given.

We have shown how to (1) derive the moment equations to any order, (2) expand the space-charge forces spatially, (3) relate the space-charge forces to the moments of the distributions, and (4) compute analytically the space-charge coefficients to any order in an expansion in nonsphericality. We have explicitly carried out all of these steps to fourth moments, including cubic terms in the forces and to cubic order in the nonsphericality; resultant equations include the effects of rf nonlinearity and have the potential for investigating equipartitioning. These equations are now being incorporated in the computer code, BEDLAM (Beam Dynamics in Linear Accelerators by Moments).

This approach to beam dynamics by moments has a number of advantages: (1) it can be systematically extended to any order, (2) a small number of equations results, (3) physically interesting and intuitive quantities are directly computed, (4) it is fully three-dimensional, (5) arbitrary external forces are allowed, (6) space charge is computed at each time step, and (7) space charge is computed quite accurately with a systematic procedure for improving the accuracy. Finally, let us note that if the external structure is periodic (a transport system), the concept of a "match" can be precisely defined; we require all moments computed to be exactly periodic. Precisely defining a match allows implementing numerically a matching procedure by a Newton technique.

Appendix

In this appendix we illustrate the derivation of moment equations in more detail.

Let us first derive Eq. (5). Multiplying Eq. (1) by x_i and integrating over phase space we obtain

$$\frac{d}{dt}\int x_i f d\vec{x}d\vec{v} + \int x_i \vec{v}\cdot\frac{\partial f}{\partial \vec{x}}\, d\vec{x}d\vec{v}$$

$$+ \frac{1}{m}\int x_i(\vec{F} + q\vec{E})\cdot\frac{\partial f}{\partial \vec{v}}\, d\vec{x}d\vec{v} = 0 \quad . \tag{A.1}$$

The first term, T_1, of Eq. (A.1) becomes

$$T_1 = N\frac{d}{dt}\langle x_i\rangle \quad . \tag{A.2}$$

In the second term, T_2, of Eq. (A.1) we can integrate by parts in $\vec{x}$ and obtain

$$T_2 = -\int v_i f d\vec{x}d\vec{v} = -N\langle v_i\rangle \quad . \tag{A.3}$$

If we do the $\vec{v}$ integration in the third term of Eq. (A.1) we find

$$\int \frac{\partial f}{\partial \vec{v}}\, d\vec{v} = f(\infty) - f(-\infty) = 0 \quad . \tag{A.4}$$

Using Eqs. (A.2), (A.3), (A.4) in Eq. (A.1) we obtain

$$\frac{d}{dt}\langle x_i\rangle - \langle v_i\rangle = 0 \quad , \tag{A.5}$$

which is just Eq. (5).

Let us derive Eq. (8). Multiplying Eq. (1) by $x_i v_j$ we get

$$\frac{d}{dt}\int x_i v_j f d\vec{x}d\vec{v} + \int x_i v_j \vec{v}\cdot\frac{\partial f}{\partial \vec{x}}\, d\vec{x}d\vec{v}$$

$$+ \int x_i v_j \frac{1}{m}(\vec{F} + q\vec{E})\cdot\frac{\partial f}{\partial \vec{v}}\, d\vec{x}d\vec{v} = 0 \quad . \tag{A.6}$$

The first term in Eq. (A.6) is just

$$N\frac{d}{dt}\langle x_i v_j\rangle \quad . \tag{A.7}$$

If we integrate by parts in $\vec{x}$ the second term, we get

$$-\int v_j v_i f d\vec{x}d\vec{v} = -N\langle v_i v_j\rangle \quad . \tag{A.8}$$

If we integrate by parts in $\vec{v}$ the third term, we get

$$-\int x_i \frac{1}{m}(F_j + qE_j) f d\vec{x}d\vec{v} = -\frac{N}{m}\langle x_i(F_j + qE_j)\rangle \quad . \tag{A.9}$$

Combining Eqs. (A.6)-(A.9) we obtain

$$\frac{d}{dt}\langle x_i v_j\rangle - \langle v_i v_j\rangle - \frac{1}{m}\langle x_i(F_j + qE_j)\rangle = 0 \quad , \tag{A.10}$$

which is the same as Eq. (8).

All the other moment equations are obtained similarly.