Lecture 3: Multi-particle Dynamics

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0.1 The KV Distribution

The Kapchinskij-Vladimirskij (KV) distribution is a self-consistent, two-dimensional distribution for which the self-fields are quadratic (i.e. the forces are linear). The distribution is applicable to long beams in transport systems where the external nonlinearities are negligible. But the distribution is unphysical since it is a δ-function in phase space. Nevertheless, it is a useful tool in the larger effort of understanding beams with space charge. Further, later we will see that the KV equations are related to rms envelope equations which have widespread applicability and are not dependent (or very weakly dependent) on the particular form of a distribution function.

A KV distribution function has the form

$$f(x, p_x, y, p_y) = \delta(Q(x, p_x, y, p_y)), \tag{1}$$

where Q is a quadratic form in (x, p_x, y, p_y). Obviously, a KV distribution transforms into a KV distribution under a linear mapping. To simplify the discussion, consider an initial distribution that is upright in phase space,

$$f^o(x, p_x, y, p_y) = C\delta(\frac{x^2}{\sigma_x^2} + \frac{p_x^2}{\lambda_x^2} + \frac{y^2}{\sigma_y^2} + \frac{p_y^2}{\lambda_y^2}). \tag{2}$$

Here σ_x, σ_y are related to the initial width of the beam in position space, and λ_x, λ_y are related to the initial width of the beam in momentum space. Also, C is a normalization constant given by

$$C = \frac{1}{\pi^2 \sigma_x \sigma_y \lambda_x \lambda_y}. \tag{3}$$

Later we will show that the space charge forces associated with a KV distribution are linear. Assuming the external forces are also linear, the beam dynamics is governed by a matrix M. For this discussion assume that the beam is propagating in a channel consisting only of drift spaces and magnetic quadrupoles. The map M is of the form

$$M = \begin{pmatrix} a_x & b_x & 0 & 0 \\ c_x & d_x & 0 & 0 \\ 0 & 0 & a_y & b_y \\ 0 & 0 & c_y & d_y \end{pmatrix}, \tag{4}$$

where $a_i d_i - b_i c_i = 1$. (We have assumed that the transport system contains only perfectly aligned quadrupoles and no skew quadrupole component. A more general analysis is straightforward but tedious.) The beam density is given by

$$\rho(x, y) = \int\int d\vec{p} f^o(M^{-1}\zeta), \tag{5}$$

or,

$$\rho(x, y) = \int\int d\vec{p}\delta\left[\frac{(d_x x - b_x p_x)^2}{\sigma_x^2} + \cdots + \frac{(-c_y y + a_y p_y)^2}{\lambda_y^2}\right]. \tag{6}$$

The integrations can be performed using the substitutions

$$\begin{aligned} q\cos\theta &= p_x\sqrt{\frac{b_x^2}{\sigma_x^2} + \frac{a_x^2}{\lambda_x^2}} - x(\frac{b_x d_x}{\sigma_x^2} + \frac{a_x c_x}{\lambda_x^2})/\sqrt{\frac{b_x^2}{\sigma_x^2} + \frac{a_x^2}{\lambda_x^2}} \\ q\sin\theta &= p_y\sqrt{\frac{b_y^2}{\sigma_y^2} + \frac{a_y^2}{\lambda_y^2}} - y(\frac{b_y d_y}{\sigma_y^2} + \frac{a_y c_y}{\lambda_y^2})/\sqrt{\frac{b_y^2}{\sigma_y^2} + \frac{a_y^2}{\lambda_y^2}} \end{aligned} \tag{7}$$

Performing the integration, we obtain

$$\rho(x,y) = \frac{1}{\pi r_x r_y} \times \left\{ \begin{array}{ll} 1 & \text{if} \quad \frac{x^2}{r_x^2} + \frac{y^2}{r_y^2} < 1 \\ 0 & \text{if} \quad \frac{x^2}{r_x^2} + \frac{y^2}{r_y^2} > 1 \end{array} \right\}, \tag{8}$$

where

$$r_x^2 = \sigma_x^2 a_x^2 + \lambda_x^2 b_x^2, \qquad r_y^2 = \sigma_y^2 a_y^2 + \lambda_y^2 b_y^2. \tag{9}$$

That is, the density is a uniformly filled ellipse with boundary given by

$$\frac{x^2}{r_x^2} + \frac{y^2}{r_y^2} = 1. \tag{10}$$

By a similar calculation, it is easy to show that every two-dimensional projection of a KV distribution is a uniformly filled ellipse.

Next we need to compute the potentials associated with this beam. An exact analytical solution is impossible because the beam envelopes, r_x and r_y, are functions of z. Following the standard approach, we will therefore compute the potentials at position z by assuming, for the potential calculation only, the r_x and r_y are constants. (Equivalently, we will neglect derivatives of the potentials with respect to z.) One can show that the scalar potential for the interior of the beam is given by

$$\psi(x,y) = \frac{-\lambda}{2\pi\epsilon_o} \left[\frac{x^2}{r_x(r_x + r_y)} + \frac{y^2}{r_y(r_x + r_y)} \right] \qquad (\frac{x^2}{r_x^2} + \frac{y^2}{r_y^2} < 1) \tag{11}$$

where λ is the charge per unit length. Note that this satisfies

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\frac{\lambda}{\pi \epsilon_o r_x r_y} \tag{12}$$

as required. Also, using

$$\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial^2 A_z}{\partial y^2} = -\mu_o \rho v_o, \tag{13}$$

we obtain

$$A_z = \frac{v_o}{c^2} \psi. \tag{14}$$

This factor will lead to the usual $1/\gamma^2$ dependence of the transverse space charge force.

Now we can compute the self-consistent Hamiltonian, i.e. one that contains both the external fields and the self-consistent space charge fields. For a quadrupole channel, including the above self-fields, we have

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{qg(z)}{2p^o}(x^2 - y^2) + \frac{q}{p^o v_o}\psi - \frac{q}{p^o} A_z. \tag{15}$$

It follows that

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{k(z)}{2}(x^2 - y^2) - K \left[\frac{x^2}{r_x(r_x + r_y)} + \frac{y^2}{r_y(r_x + r_y)} \right] \tag{16}$$

where

$$k(z) = \frac{q}{p^o} g(z), \tag{17}$$

and where

$$K = \frac{q\lambda}{2\pi\epsilon_o p^o v_o \gamma_o^2} \tag{18}$$

is the so-called generalized perveance.

Using the properties of the linear transfer maps (lecture notes 01),

$$\frac{dM}{dt} = JSM, \tag{19}$$

where S is a symmetric matrix defined in terms of H_2 according to

$$H_2 = \frac{1}{2}\sum_{a,b=1}^{2m} S_{ab}\zeta_a\zeta_b. \tag{20}$$

we can determine that the matrix S associated with this Hamiltonian is

$$S = \begin{pmatrix} s_{11} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & s_{33} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{21}$$

where

$$\begin{aligned} s_{11} &= k - \frac{2K}{r_x(r_x+r_y)} \\ s_{33} &= -k - \frac{2K}{r_y(r_x+r_y)} \end{aligned} \tag{22}$$

$$\tag{23}$$

Using the equation $M' = JSM$, we obtain 8 first order differential equations for the matrix elements of M:

$$\begin{array}{cc} a_x' = c_x & a_y' = c_y \\ b_x' = d_x & b_y' = d_y \\ c_x' = -a_x\left[k - \frac{2K}{r_x(r_x+r_y)}\right] & c_y' = -a_y\left[-k - \frac{2K}{r_y(r_x+r_y)}\right] \\ d_x' = -b_x\left[k - \frac{2K}{r_x(r_x+r_y)}\right] & d_y' = -b_y\left[-k - \frac{2K}{r_y(r_x+r_y)}\right] \end{array} \tag{24}$$

These can be combined into four second order equations,

$$\begin{aligned} a_x'' + a_x\left[k - \frac{2K}{r_x(r_x+r_y)}\right] &= 0, \\ b_x'' + b_x\left[k - \frac{2K}{r_x(r_x+r_y)}\right] &= 0, \\ a_y'' + a_y\left[-k - \frac{2K}{r_y(r_x+r_y)}\right] &= 0, \\ b_y'' + b_y\left[-k - \frac{2K}{r_y(r_x+r_y)}\right] &= 0. \end{aligned} \tag{25}$$

Summarizing, we have shown that a KV distribution with initial value $f^o(\zeta)$ evolves according to $f^o(M^{-1}\zeta)$, where the matrix elements of M satisfy the above equations. Lastly, we can now obtain

the KV envelope equations. Recall that $r_x^2 = \sigma_x^2 a_x^2 + \lambda_x^2 b_x^2$, and similarly for r_y^2. Differentiating these equations twice with respect to z, and making use of the previous equations for the matrix elements of M, we obtain, after some manipulation,

$$\begin{aligned} r_x'' + kr_x - \frac{2K}{(r_x + r_y)} - \epsilon_x^2/r_x^3 &= 0, \\ r_y'' - kr_y - \frac{2K}{(r_x + r_y)} - \epsilon_y^2/r_x^3 &= 0, \end{aligned} \tag{26}$$

where ϵ_x and ϵ_y denote the edge emittances

$$\begin{aligned} \epsilon_x &= \sigma_x \lambda_x, \\ \epsilon_y &= \sigma_y \lambda_y. \end{aligned} \tag{27}$$

These are the well-known KV envelope equations.

It is worth noting that we could have started this discussion by assuming a more general initial distribution. For example, we could have considered

$$f^o(x, p_x, y, p_y) = C\delta(\frac{x^2}{\sigma_x^2} + \frac{2\mu_x}{\sigma_x \lambda_x} x p_x + \frac{p_x^2}{\lambda_x^2} + \frac{y^2}{\sigma_y^2} + \frac{2\mu_y}{\sigma_y \lambda_y} y p_y + \frac{p_y^2}{\lambda_y^2}), \tag{28}$$

where

$$C = \frac{\sqrt{1-\mu_x^2}\sqrt{1-\mu_y^2}}{\pi^2 \sigma_x \sigma_y \lambda_x \lambda_y}. \tag{29}$$

In this case, we would have ended up with the same KV equations as above. The only difference is that the edge emittances would be given by

$$\begin{aligned} \epsilon_x &= \frac{\sigma_x \lambda_x}{\sqrt{1-\mu_x^2}}, \\ \epsilon_y &= \frac{\sigma_y \lambda_y}{\sqrt{1-\mu_y^2}}. \end{aligned} \tag{30}$$

0.2 RMS Equations

RMS envelope equations were first introduced by Sacherer and Lapostolle [1] [2]. An extensive treatment of cylindrically symmetric systems was given by Lee and Cooper [3]. In many situations, envelope equations provide a useful description of charged particle beams. As we will see below, the 2D equations look identical to the KV envelope equations. A key difference, however, is that the rms equations are meant to be applicable to *all* distributions, not just KV distributions. Furthermore, it is remarkable that, under certain assumptions (namely elliptical symmetry in the 2D case), the rms equations are *exact*; there are no terms whose values depend on the type of distribution function being modeled. They are the same whether one is modeling a KV distribution, a Gaussian distribution, or any other distribution. Also, even in the 3D case, for beams with ellipsoidal symmetry, they are only *weakly* dependent on the type of distribution. Unfortunately the rms equations have a notable shortcoming: they contain terms that involve the rms emittances, whose time-dependence are generally not known *apriori*. Thus, in this sense the rms envelope description of beams is not a *closed* description. However, they are extremely useful in those cases where the emittances change

little or not at all. Furthermore, since the rms equations involve only a small number of ordinary differential equations, they can be integrated quickly, and they provide an excellent starting point in the design and optimization of beam lines.

For the sake of this discussion, consider a particle beam propagating in a quadrupole channel. Suppose that the beam is long compared with its transverse dimensions, and that we can neglect any longitudinal variation when calculating the beam self-fields. We will neglect image charge effects, and we will suppose that the beam is launched along the axis of a perfectly aligned transport system. We will use the longitudinal coordinate, z, as the independent variable. The canonical coordinates and momenta for the transverse phase space are denoted (x, p_x, y, p_y). Let the vector potential associated with the quadrupoles be given by

$$A_x = A_y = 0, \tag{31}$$

$$A_z = \frac{1}{2} g(z)(y^2 - x^2), \tag{32}$$

where $g(z)$ denotes the magnetic quadrupole gradient. Let Ψ denote the scalar potential associated with the self-fields and, neglecting transverse currents, suppose that the associated vector potential is given by

$$A_x = A_y = 0, \tag{33}$$

$$A_z = \frac{\beta_o}{c}\Psi, \tag{34}$$

where $\beta_o c$ is the velocity on the design trajectory. Rather than working with the variables (x, p_x, y, p_y) it is convenient to define dimensionless variables $(\bar{x}, \bar{p}_x, \bar{y}, \bar{p}_y)$ according to

$$\bar{x} = x/l, \qquad \bar{p}_x = p_x/p_o, \tag{35}$$

$$\bar{y} = y/l, \qquad \bar{p}_y = p_y/p_o, \tag{36}$$

where p_o denotes the momentum on the design trajectory (*i.e.* $p_o = \gamma_o \beta_o mc$) and where l is a scale length. The Hamiltonian (in MKSA units) governing these variables is given approximately by

$$H(\bar{x}, \bar{p}_x, \bar{y}, \bar{p}_y; z) = \frac{1}{2l}(\bar{p}_x^2 + \bar{p}_y^2) + \frac{lk(z)}{2}(\bar{x}^2 - \bar{y}^2) + \frac{K/2}{l}\hat{\Psi}(l\bar{x}, l\bar{y}, z), \tag{37}$$

where

$$k(z) = (q/p_o)g(z), \tag{38}$$

and where K is the generalized perveance,

$$K = \frac{qI}{2\pi\epsilon_o p_o v_o^2 \gamma_o^2}. \tag{39}$$

Also, $\hat{\Psi}$ is related to Ψ according to

$$\Psi = \frac{\lambda}{4\pi\epsilon_o}\hat{\Psi}, \tag{40}$$

where λ is the charge per unit length measured in the lab frame, $\lambda = I/v_o$. Note that we have expanded the relativistic Hamiltonian to second order in the phase space variables, with the exception of the scalar potential, as is the standard procedure for deriving rms envelope equations. For

the remainder of the discussion of two dimensional systems we will set $l = 1$ m, and we will drop the overbar on $(\bar{x}, \bar{p}_x, \bar{y}, \bar{p}_y)$. The Hamiltonain now appears as

$$H(x, p_x, y, p_y; z) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{k(z)}{2}(x^2 - y^2) + \frac{K}{2}\hat{\Psi}(lx, ly, z), \tag{41}$$

and the resulting equations of motion are

$$\begin{aligned} x' &= p_x, & (42)\\ p_x' &= -kx - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial x}, & (43)\\ y' &= p_y, & (44)\\ p_y' &= ky - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial y}, & (45) \end{aligned}$$

where a prime denotes d/dz.

0.2.1 Derivation of RMS Equations

Let X and Y denote the rms envelopes,

$$\begin{aligned} X &= \sqrt{< x^2 >}, \\ Y &= \sqrt{< y^2 >}, \end{aligned} \tag{46}$$

where $<>$ denotes an average over the distribution function. Consider, for example, the evolution of X:

$$X' = \frac{< xx' >}{\sqrt{< x^2 >}} = \frac{< xp_x >}{X}. \tag{47}$$

Differentiating again, we obtain

$$X'' = -\frac{< xp_x > X'}{X^2} + \frac{< x'p_x + xp_x' >}{X}. \tag{48}$$

After some manipulation we obtain

$$X'' = \frac{< xp_x' >}{X} + \frac{\epsilon_x^2}{X^3}, \tag{49}$$

where the horizontal rms emittance is given by

$$\epsilon_x^2 =< x^2 >< p_x^2 > - < xp_x >^2 . \tag{50}$$

Substituting Eq. (43), we obtain

$$X'' + kX + \frac{(K/2)}{X} < x\frac{\partial\hat{\Psi}}{\partial x} > -\frac{\epsilon_x^2}{X^3} = 0. \tag{51}$$

All that remains is to compute $< x\frac{\partial\hat{\Psi}}{\partial x} >$. To do this, we will follow Sacherer [1] and assume that the beam density has elliptical symmetry:

$$\rho(x, y) = \rho\left(\frac{x^2}{a^2} + \frac{y^2}{b^2}\right). \tag{52}$$

Before continuing, we note some properties of ρ. Assuming that ρ is normalized to unity,

$$\int_{-\infty}^{\infty} dx\ dy\ \rho\left(\frac{x^2}{a^2}+\frac{y^2}{b^2}\right)=1, \tag{53}$$

it follows that

$$ab\int_0^{\infty} 2\pi r\ dr\ \rho(r^2)=1. \tag{54}$$

By a similar calculation,

$$\begin{aligned}\sqrt{<x^2>} &= aC,\\ \sqrt{<y^2>} &= bC,\end{aligned} \tag{55}$$

where

$$C=\pi ab\int_0^{\infty} r^3\ dr\ \rho(r^2). \tag{56}$$

That is, a and b are proportional to the rms beam sizes, with the same proportionality constant for both.

Now consider Poisson's equation,

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}=-\lambda\rho/\epsilon_o, \tag{57}$$

where, as mentioned previously, λ is the charge per unit length. Given the distribution (52), we can write the solution of Poisson's equation formally as,

$$\Psi=-\frac{ab}{4\epsilon_o}\int_0^{\infty} ds\ \frac{\eta\left(\frac{x^2}{a^2+s}+\frac{y^2}{b^2+s}\right)}{\sqrt{a^2+s}\sqrt{b^2+s}}, \tag{58}$$

where the derivative of η with respect to its argument is ρ. It follows that

$$<x\frac{\partial\hat{\Psi}}{\partial x}>=-2\pi ab\int_{-\infty}^{\infty}dx\ \int_{-\infty}^{\infty}dy\ \int_0^{\infty}ds\ \frac{x^2\rho\left(\frac{x^2}{a^2+s}+\frac{y^2}{b^2+s}\right)}{(a^2+s)^{3/2}(b^2+s)^{1/2}}\rho\left(\frac{x^2}{a^2}+\frac{y^2}{b^2}\right) \tag{59}$$

Now make the change of variables $(x,y)\leftrightarrow(r,\theta)$,

$$\begin{aligned}r\cos\theta &= \frac{x}{\sqrt{a^2+s}},\\ r\sin\theta &= \frac{y}{\sqrt{b^2+s}},\end{aligned} \tag{60}$$

followed by another change of variables $s\leftrightarrow r'$,

$$r'^2=r^2\left[1+s\left(\frac{\cos^2\theta}{a^2}+\frac{\sin^2\theta}{b^2}\right)\right]. \tag{61}$$

Performing the integration of θ, and making use of the relation

$$\int_0^{2\pi}d\theta\ \frac{\cos^2\theta}{\frac{\cos^2\theta}{a^2}+\frac{\sin^2\theta}{b^2}}=2\pi ab\frac{a}{a+b}, \tag{62}$$

we obtain

$$< x\frac{\partial\hat{\Psi}}{\partial x} >= \frac{-2a^3b^2}{a+b}\int_0^\infty dr\ \rho(r^2)2\pi r\int_r^\infty dr'\ \rho(r'^2)2\pi r'. \tag{63}$$

Now define a quantity $F(r)$ according to

$$F(r) = ab\int_0^r \rho(r^2)2\pi r\ dr, \tag{64}$$

where, from Eq. (54), $F(\infty) = 1$. Then we can write

$$< x\frac{\partial\hat{\Psi}}{\partial x} >= -2\frac{a}{a+b}\int_0^\infty dr\ \frac{dF}{dr}\left(1 - F(r)\right). \tag{65}$$

This can be integrated to yield

$$< x\frac{\partial\hat{\Psi}}{\partial x} >= \frac{-a}{a+b} = \frac{-X}{X+Y}, \tag{66}$$

where we have used Eqs. (55) in the final equality. It follows that the rms envelope equations for a beam in a quadrupole channel are given by [1, 2]

$$\begin{aligned}
&\frac{d^2X}{dz^2} + kX - \frac{K/2}{X+Y} - \frac{\mathcal{E}_x^2}{X^3} = 0,\\
&\frac{d^2Y}{dz^2} - kY - \frac{K/2}{X+Y} - \frac{\mathcal{E}_y^2}{Y^3} = 0,
\end{aligned} \tag{67}$$

where $\mathcal{E}_x$ and $\mathcal{E}_y$ denote unnormalized rms emittances. Since these are rms equations the factor in the space charge term is $K/2$, whereas it would be $2K$ for the KV equations. In closing, we note that the envelope equations are derivable from a Hamiltonian, $H^{\rm env}$, where

$$H^{\rm env}(X, P_x, Y, P_y) = \frac{1}{2}(P_x^2 + \frac{\mathcal{E}_x^2}{X^2}) + \frac{1}{2}(P_y^2 + \frac{\mathcal{E}_y^2}{Y^2}) + \frac{k}{2}(X^2 - Y^2) - (K/2)\log(X+Y). \tag{68}$$

Lastly, one can use the envelope Hamiltonian to define depressed phase advances, μ_x and μ_y, of a particle in an equivalent KV beam. Referring to the envelope Hamiltonian, we regard the phase advances as coordinates and the emittances as a canonically conjugate momenta. (Since the phase advance appears nowhere in the Hamiltonian, the emittance is constant, as expected). Taking this view, we obtain

$$\begin{aligned}
\mu_x = &\quad \mathcal{E}_x\int\frac{dz}{X^2},\\
\mu_y = &\quad \mathcal{E}_y\int\frac{dz}{Y^2}.
\end{aligned} \tag{69}$$

For a KV distribution, these formulas apply to all the particles in the beam (since the forces are linear). For other distributions they apply to the equivalent KV beam (*i.e.* a KV beam with the same rms values). The phase advance equations can be integrated along with the envelope equations.

0.3 Particle Simulation Techniques

0.3.1 Overview

Particle simulation techniques are widely used in the computational cosmology, plasma physics, and accelerator physics communities. In all three cases the interaction between the particles varies as $1/r^2$. What sets distinguishes them is the sign of the force and the boundary conditions. In regard to cosmology, N-body simulations are shedding light on the formation of large scale structure in the universe. In these simulations the force is the gravitational force, which is attractive. The phenomenon on "clumping," i.e. the formation of structure on a sub-grid scale due to the attractive nature of the force, is an important issue in these simulations. In regard to plasma simulation and accelerator simulation, the force between particles is the electromagnetic force, which is repulsive. The main difference between these simulations is the boundary conditions and the externally applied forces. The boundary conditions are quite different for, say, a tokamak, than for a linac. Also, the external forces in accelerators have a unique and complicated dependence on the independent variable, (e.g. the z-coordinate) due to the fact that beamline elements such as focusing magnets and accelerating gaps are physically localized objects that are separated along the beamline.

Particle simulations are an important tool for designing high-current machines where where the beam self-fields must be considered in addition to the externally applied fields. Two obvious examples are high-current rf linacs and induction linacs. Though envelope calculations provide some means of modeling these systems, that treatment cannot provide a detailed description of the beam evolution, and an envelope description is really only useful when the emittance growth is small (which is possible) or known *apriori* (which is almost never the case).

Suppose we want to model an intense beam in a quadrupole or solenoid channel. The self-fields in this problem are essentially electrostatic. Though the beam itself might be moving at a relativistic velocity, the motion of particles around the reference trajectory is not relativistic. Essentially, we can solve the self-consistency problem by simply solving Poisson's equation in the beam frame and then doing a Lorentz transformation back to the lab frame. Thus, this problem is identical to the treatment of quadupoles in lecture two, except that now there are self-potentials, Ψ^{self} and A^{self}, that have to be considered. The usual procedure is to expand the Hamiltonian,

$$\begin{aligned} H(X,P_x,Y,P_y,T,P_t) &= -\tfrac{q}{\delta l}A_z \\ -\tfrac{1}{l}\left[(\tfrac{\omega l}{c}P_t+\tfrac{\omega l}{c}\bar{p}_t^g+\tfrac{q}{\delta c}\psi)^2-(\tfrac{mc}{\delta})^2-(P_x+\bar{p}_x^g-\tfrac{q}{\delta}A_x)^2-(P_y+\bar{p}_y^g-\tfrac{q}{\delta}A_y)^2\right]^{1/2} \\ -\tfrac{d\bar{x}^g}{dz}(P_x+\bar{p}_x^g)+\tfrac{d\bar{p}_x^g}{dz}X-\tfrac{d\bar{y}^g}{dz}(P_y+\bar{p}_y^g)+\tfrac{d\bar{p}_y^g}{dz}Y-\tfrac{d\bar{t}^g}{dz}(P_t+\bar{p}_t^g)+\tfrac{d\bar{p}_t^g}{dz}T \end{aligned} \tag{70}$$

and keep one power of Ψ^{self}. Also, the vector potential associated with the beam has only a z-component (for transport systems where the beam is moving in a straight line along the z-axis), which causes the beam to have a self-magnetic field, B_θ. The vector potential can be found by performing a Lorentz transformation, the result being

$$A_z^{self}=\frac{\beta_o}{c}\Psi^{self} \tag{71}$$

in MKSA units. Upon expanding Eq. (**??**), the two terms involving Ψ^{self} and A_z^{self} can be combined into a single term. The result, for a quadrupole system, is

$$H(\bar{x},\bar{p}_x,\bar{y},\bar{p}_y,z)=\frac{1}{2l}(\bar{p}_x^2+\bar{p}_y^2)+\frac{lk(z)}{2}(\bar{x}^2-\bar{y}^2)+\frac{K/2}{l}\hat{\Psi}(l\bar{x},l\bar{y},z), \tag{72}$$

where

$$k(z) = (q/p_o)g(z), \tag{73}$$

where K is the generalized perveance,

$$K = \frac{qI}{2\pi\epsilon_o p_o v_o^2 \gamma_o^2}. \tag{74}$$

and where $\hat{\Psi}$ is related to Ψ^{self} according to

$$\Psi^{\text{self}} = \frac{\lambda}{4\pi\epsilon_o}\hat{\Psi}. \tag{75}$$

In the above, λ is the charge per unit length measured in the lab frame, $\lambda = I/v_o$. For the remainder of this discussion we will set the scale length, $l = 1$ m.

We can implement a time-stepping algorithm for the simulation of intense beams using the same techniques as presented earlier for single-particle dynamics. In particular, we can use split-operator methods, separating terms associated with the externally applied fields from those associated with the self fields:

$$H = H_{ext} + H_{self} \tag{76}$$

The Hamiltonian, H_{ext}, for the external fields was dealt with in lecture 2. In the linear approximation, we have already calculated the map, M_{ext}, applicable to quadrupole channels. The new feature in the simulation of intense beams is the term H_{self},

$$H_{self} = \frac{K}{2}\hat{\Psi}(x, y). \tag{77}$$

Since this depends only on coordinates and not momenta, we can write down the map immediately:

$$\begin{aligned} x^{fin} &= x^{in}, \\ p_x^{fin} &= p_x^{in} - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial x}, \\ y^{fin} &= y^{in}, \\ p_y^{fin} &= p_y^{in} - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial y}. \end{aligned} \tag{78}$$

In other words, the map M_{self} provides a "space charge kick" to the particles.

All that remains is to compute the scalar potential Ψ, or to compute the self-fields E_x and E_y directly. This is the major task in implementing a particle simulation.

0.4 Grid-Based Techniques

The situation becomes considerably more complicated when we consider beams without azimuthal symmetry, and various boundary conditions. If one wants to use a large number of particles, then it is hopeless to use a direct n-body approach in which one adds together all the interparticle forces. The amount of data and number of arithmetic operations required goes as $O(N^2)$, where N is the number of particles in the simulation. Roughly speaking, a three-dimensional, double precision simulation with 10^4 particles would require a few GBytes of memory (which is now possible), but a simulation with 10^5 particles would require 100 times that amount. Fortunately, many algorithms have been developed to solve Poisson's equation that do not have the $O(N^2)$ dependency.

One approach, which will will describe here, is to place the charges on a numerical grid and solve the field equations on the grid. The steps required are the following:

1. **Charge Deposition:** Place charges on a numerical grid.
2. **Field Solution:** Solve the field equations on the grid.
3. **Field Interpolation:** Interpolate the fields at the particle positions based on values at the grid locations.

The name "Particle-In-Cell" is used in many contexts, but it is often associated with a hierarchy of schemes that begins with "Nearest Grid Point" (NGP), "Cloud In Cell" (CIC), and "Triangular Shaped Charge" (TSC). We will describe the first two here. Further information can be found in the literature [4].

0.4.1 Charge Assignment and Field Interpolation

In the Nearest Grid Point scheme, all the charge associated with a given particle is deposited on a single grid point, namely the one nearest the particle, in the charge deposition phase. Similarly, during the interpolation phase, the field at a given particle is taken to be the field at the grid point nearest the particle.

In the 2D, Cloud In Cell scheme, the charge associated with a given particle is deposited on 4 mesh points that make up the vertices of a square or rectangle surrounding a particle. (Similarly, in 3D, the charge is deposited on the 8 vertices of a cube.) The amount of charge deposited on each vertex is called the weight, and the sum of the weights is equal to one. The same weights are normally used during the interpolation phase to compute the interpolated field value at particle positions.

0.4.2 Isolated Systems

Hockney's convolution algorithm for calculating the potential of isolated systems is described in [4]. Its main drawback is that it involves doubling the grid size in all dimensions. However, with some effort the increased memory requirement can be partly ameliorated. The advantage of the Hockney method is that, while some people move the boundaries "sufficiently far" from the charge distribution so that they are not an issue, in the Hockney algorithm the boundaries are analytically moved off to infinity. Also, since it involves the use of Fast Fourier Transforms, the method is reasonably fast. We will demonstrate the validity of this approach in one dimension. The extension to higher dimensions is straightforward.

Consider the problem of evaluating the sums

$$Y_l = \sum_{n=0}^{N-1} h_n X_{l-n} \qquad l = 0, \ldots, N-1 \tag{79}$$

where X_l is *not* periodic. Such sums arise when one discretizes the formal solution of the Poisson equation in free space,

$$\psi(\vec{x}) = \int d\vec{x}' \; \rho(\vec{x}) \; G(\vec{x} - \vec{x}'). \tag{80}$$

Here X_{l-n} corresponds to the Green function, h_n corresponds to the charge density, and Y_l corresponds to the scalar potential. If X_l were periodic, Eq. (78) would be a *circular convolution*, and we could use Fast Fourier Transform techniques to solve the problem in $O(N \log N)$ steps instead of $O(N^2)$ steps.

Hockney's algorithm requires that all of the source terms, h_n, reside in half of the mesh called the *physical region*. We will show that we can replace Eq. (78) by a circular convolution that matches (78) in the physical region; in the other half of the mesh (the unphysical region) the potential is calculated incorrectly, and must be discarded. To see how this works, assume there are no sources in the unphysical region,

$$h_n = 0 \qquad \frac{N}{2} \le n \le N-1. \tag{81}$$

Define a periodic Green function χ_l, by

$$\begin{aligned} \chi_l &= X_l \qquad -\frac{N}{2} \le l \le \frac{N}{2} - 1, \\ \chi_{l+N} &= \chi_l. \end{aligned} \tag{82}$$

Now consider the sum

$$\hat{Y}_l = \frac{1}{N} \sum_{k=0}^{N-1} W^{-lk} \Big(\sum_{n=0}^{N-1} h_n W^{nk}\Big)\Big(\sum_{m=0}^{N-1} \chi_m W^{mk}\Big) \qquad 0 \le l \le N-1, \tag{83}$$

where $W = \exp(-2\pi i/N)$. We claim that

$$\hat{Y}_l = Y_l \qquad 0 \le l \le \frac{N}{2} - 1. \tag{84}$$

Proof: By Eq. (80)

$$\hat{Y}_l = \sum_{n=0}^{N/2-1} \sum_{m=0}^{N-1} h_n \chi_m \frac{1}{N} \sum_{k=0}^{N-1} W^{(m+n-l)k}. \tag{85}$$

Now use the relation

$$\sum_{k=0}^{N-1} W^{(m+n-l)k} = N\delta_{m+n,l+jN} \qquad (j \text{ an integer}). \tag{86}$$

It follows that

$$\hat{Y}_l = \sum_{n=0}^{N/2-1} h_n \; \chi_{l-n+jN}. \tag{87}$$

But χ is periodic with period N. Thus,

$$\hat{Y}_l = \sum_{n=0}^{N/2-1} h_n \; \chi_{l-n} = \sum_{n=0}^{N/2-1} h_n \; X_{l-n} \quad \text{if} \quad -\frac{N}{2} \le l-n \le \frac{N}{2} - 1 \tag{88}$$

That is,

$$\hat{Y}_l = Y_l \tag{89}$$

if

$$-\frac{N}{2} + n \le l \le \frac{N}{2} - 1 + n \tag{90}$$

and, from Eq. (87),

$$0 \le n \le N/2 - 1. \tag{91}$$

But Eqs. (89) and (90) are clearly satisfied for

$$0 \le l \le N/2 - 1, \tag{92}$$

so the proof is complete.

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