Computational Methods in Accelerator Physics

Robert D. Ryne

Contents

Chapter 1

Single Particle Dynamics and Numerical Integration

1.1 Lagrangian and Hamiltonian Dynamics

In accelerator physics and magnetic optics, one is interested in the motion of charged particles in electromagnetic fields. One way of describing the dynamics is through the Lorentz force equations. For a particle of charge q and mass m, they are given in MKSA units by

$$\frac{d\vec{p}^{\,\mathrm{mech}}}{dt} = q\vec{E} + q\vec{v} \times \vec{B}, \tag{1.1}$$

where $\vec{v}$ is the particle's velocity, and where $\vec{E}$ and $\vec{B}$ are the electric and magnetic field, respectively. The quantity $\vec{p}^{\,\mathrm{mech}}$ denotes the mechanical momentum, which is given in Cartesian coordinates by

$$\vec{p}^{\,\mathrm{mech}} = \gamma m \vec{v}, \tag{1.2}$$

where $\gamma = \sqrt{1-\beta^2}$, $\beta^2 = \vec{\beta} \cdot \vec{\beta}$, and $\vec{\beta} = \vec{v}/c$. The dynamics described by the Lorentz force equation can be reformulated in terms of Lagrange's equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \tag{1.3}$$

where $L(\vec{q}, \dot{\vec{q}}_i, t)$ denotes the Lagrangian, $\vec{q} = (q_1, q_2, \ldots)$ denotes a set of generalized coordinates, and where a dot denotes d/dt. For a charged particle in electromagnetic fields,

$$L = -mc^2\sqrt{1-\beta^2} - q\psi + q\vec{v}\cdot\vec{A}, \tag{1.4}$$

where $\psi(\vec{x}, t)$ and $\vec{A}(\vec{x}, t)$ are the scalar and vector potentials, respectively. In MKSA units, these are related to the electric and magnetic field according to

$$\vec{B} = \nabla \times \vec{A}, \tag{1.5}$$

$$\vec{E} = -\nabla\psi - \frac{\partial \vec{A}}{\partial t}. \tag{1.6}$$

- **Problem 1.1**
  Using Cartesian coordinates $\vec{q} = (x, y, z)$, verify that Lagrange's equations with Lagrangian (1.4) reproduce the Lorentz force equations. (Hint: use the relation $\frac{d}{dt} = \frac{\partial}{\partial t} + v \cdot \nabla$).

In all that follows we will use the Hamiltonian formulation of charged particle dynamics. To do this, introduce the canonical momentum, p_i, which is conjugate to the generalized coordinate, q_i,

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}. \tag{1.7}$$

The Hamiltonian $H(\vec{q}, \vec{p}, t)$ is related to the Lagrangian, $L(\vec{q}, \dot{\vec{q}}, t)$ according to

$$H(\vec{q}, \vec{p}, t) = \sum_i p_i \dot{q}_i - L, \tag{1.8}$$

where Eq. (1.7) is used to reexpress $\dot{q}_i$ in terms of p_i. Hamilton's equations are given by

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{1.9}$$

It follows from Eq. (1.7) and Eq. (1.4) that, in Cartesian coordinates, the canonical momenta are given by

$$\vec{p} = \gamma m \vec{v} + q\vec{A} = \vec{p}^{\,\mathrm{mech}} + q\vec{A}. \tag{1.10}$$

(In these notes we will use the convention that, unless it is specifically stated or annotated otherwise, a quantity p denotes a *canonical* momentum.) It follows that the Hamiltonian for a particle of mass m and charge q, in Cartesian coordinates, is given by

$$H = \left[m^2c^4 + c^2(\vec{p} - q\vec{A})^2\right]^{1/2} + q\psi. \tag{1.11}$$

Of course, this is just the total energy, $\sqrt{(p^{\rm mech})^2c^2 + m^2c^4} + q\psi$.

- **Problem 1.2**
  Verify that the Hamiltonian, (1.11), follows from Eqs. (1.8), (1.4), and (1.10).

- **Problem 1.3**
  In cylindrical coordinates (r, θ, z) the velocity vector is given by $\vec{v} = \dot{r}\ \hat{r} + r\dot{\theta}\ \hat{\theta} + \dot{z}\ \hat{z}$, where $(\hat{r}, \hat{\theta}, \hat{z})$ are unit vectors. Using this, along with $\vec{A} = (A_r, A_\theta, A_z)$ in Eq. (1.4), and Eq. (1.7), show that the canonical momenta and resulting Hamiltonian are given by

$$\begin{aligned} p_r &= \gamma m\dot{r} + qA_r \\ p_\theta &= \gamma m r^2\dot{\theta} + qrA_\theta \\ p_z &= \gamma m\dot{z} + qA_z \end{aligned} \tag{1.12}$$

$$H = \left[m^2c^4 + c^2(p_r - qA_r)^2 + c^2(p_\theta/r - qA_\theta)^2 + c^2(p_z - qA_z)^2\right]^{1/2} + q\psi. \tag{1.13}$$

Now we will introduce a key concept in our approach to analyzing charged particle dynamics in accelerators and beam transport systems: the notion of a *transfer map*. Let $H(\zeta, t)$ denote the Hamiltonian of some dynamical system, where $\zeta = (q_1, p_1, q_2, p_2, \ldots, q_m, p_m)$. The $2m$-dimensional space whose axes are $q_1, p_1, q_2, p_2, \ldots, q_m, p_m$ is called *phase space*. The $2m+1$ dimensional space that is the direct product of phase space with the time axis is called *state space*. As a particle evolves in time, its trajectory traces out a path in state space (and also in phase space). If we choose some initial time, t^{in}, and some final time, $t^{\rm fin}$, then Hamilton's equations may be regarded as defining a generally nonlinear

mapping, $\mathcal{M}$, that maps $\zeta(t^{\rm in})$ into $\zeta(t^{\rm fin})$. We will use the notation $\zeta^{\rm in} = \zeta(t^{\rm in})$ and $\zeta^{\rm fin} = \zeta(t^{\rm fin})$, and we will write

$$\zeta^{\rm fin} = \mathcal{M}\zeta^{\rm in}. \tag{1.14}$$

The quantity $\mathcal{M}$ is called the *transfer map* relating $\zeta^{\rm in}$ and $\zeta^{\rm fin}$. It will turn out that, because $\mathcal{M}$ comes from a Hamiltonian, it belongs to the class of mappings known as *symplectic* mappings. Properties of symplectic mappings will be discussed in detail later.

1.1.1 Coordinate as an Independent Variable

To study beam transport systems it is often useful to choose a coordinate as the independent variable, rather than the time. For example, in systems where the design orbit is a straight line (call it the z-axis), one could choose the coordinate z as the independent variable. To do this, define a new variable, p_t, by

$$p_t = -H(\vec{q}, \vec{p}, t). \tag{1.15}$$

In other words, p_t is just the negative of the single particle total energy. Next, invert the above equation to obtain p_z as a function of (x, p_x, y, p_y, t, p_t) and z. By the Implicit Function Theorem, we can do this so long as $\partial H/\partial p_z \neq 0$ in the region of interest (i.e. so long as $\dot{z}$ is nonzero). Lastly, define a quantity K according to

$$K(x, p_x, y, p_y, t, p_t; z) = -p_z. \tag{1.16}$$

Then it is easy to show (by the chain rule) that

$$x' = \frac{\partial K}{\partial p_x} \quad , \qquad p_x' = -\frac{\partial K}{\partial x}, \tag{1.17}$$

$$y' = \frac{\partial K}{\partial p_y} \quad , \qquad p_y' = -\frac{\partial K}{\partial y}, \tag{1.18}$$

$$t' = \frac{\partial K}{\partial p_t} \quad , \qquad p_t' = -\frac{\partial K}{\partial t}, \tag{1.19}$$

where a prime denotes d/dz. In other words, K is the new Hamiltonian with z as the independent variable. The new Hamiltonian is given by

$$K(x, p_x, y, p_y, t, p_t; z) = -\left[(p_t + q\psi)^2/c^2 - m^2c^2 - (p_x - qA_x)^2 - (p_y - qA_y)^2\right]^{1/2} - qA_z. \tag{1.20}$$

Similarly, if we use θ as the independent variable in cylindrical coordinates, it follows that

$$K(r, p_r, z, p_z, t, p_t; \theta) = -r\left[(p_t + q\psi)^2/c^2 - m^2c^2 - (p_r - qA_r)^2 - (p_z - qA_z)^2\right]^{1/2} - qrA_\theta. \tag{1.21}$$

Most of our examples that follow will utilize z as the independent variable. However, when discussing formalism one often uses the symbol t in a generic sense to denote the independent variable. The reader should keep in mind that, when we say "time-dependent" we often mean "z-dependent," and references to $t^{\rm in}$ and $t^{\rm fin}$ (initial and final times) often mean $z^{\rm in}$ and $z^{\rm fin}$.

1.1.2 Canonical Transformations

In what follows it will prove useful to perform various canonical transformations from one set of variables, $(\vec{q}, \vec{p})$, to new variables, $(\vec{Q}, \vec{P})$. Concurrently, the original Hamiltonian, $H(\vec{q}, \vec{p})$, will be transformed into a new Hamiltonian $H^{\rm new}(\vec{Q}, \vec{P})$. For a general discussion, see, e.g., Goldstein [1]. For our purposes, two types of transforms will be used frequently.

First consider a scaling transformation, for which

$$Q_i = q_i/a_i, \qquad P_i = p_i/b_i \qquad (i = 1, 2, 3), \tag{1.22}$$

where a_i and b_i are constants. It is easy to show that, so long as the product $a_i b_i \equiv ab$ is the same for all i, the transformation is canonical, and the new Hamiltonian is given by

$$H^{\rm new}(\vec{Q}, \vec{P}) = \frac{1}{ab} H(a\vec{Q}, b\vec{P}). \tag{1.23}$$

Next consider a canonical transformation based on the following generating function,

$$F_2(\vec{q}, \vec{P}, t) = (x - x^g)(P_x + p_x^g) + (y - y^g)(P_y + p_y^g) + (z - z^g)(P_z + p_z^g), \tag{1.24}$$

where $x^g, p_x^g, y^g, p_y^g, z^g, p_z^g$ are functions of t. Based on this generating function, the new variables are related to the old variables according to

$$\vec{Q} = \frac{\partial F_2}{\partial \vec{P}}, \qquad \vec{p} = \frac{\partial F_2}{\partial \vec{q}}, \tag{1.25}$$

and the new Hamiltonian is given by

$$H^{\rm new}(\vec{Q},\vec{P}) = H + \frac{\partial F_2}{\partial t}. \tag{1.26}$$

In this case, we obtain

$$\begin{aligned} X = x - x^g, \qquad P_x &= p_x - p_x^g, \\ Y = y - y^g, \qquad P_y &= p_y - p_y^g, \\ Z = z - z^g, \qquad P_z &= p_z - p_z^g. \end{aligned} \tag{1.27}$$

- **Problem 1.4**
  Show that Eqs. (1.24) and (1.25) lead to (1.27).

Lastly, suppose that $(x^g, p_x^g, y^g, p_y^g, z^g, p_z^g)$ denotes a particular solution of Hamilton's Equations with Hamiltonian H, which we will call a reference trajectory. Then, from Eq. (1.27), the new variables are deviations from the reference trajectory. Furthermore, one can show that the new Hamiltonian, $H^{\rm new}(\vec{Q},\vec{P},t)$, if expanded in the new variables, will contain no linear terms.

- **Problem 1.5**
  Verify that, if $H^{\rm new}(\vec{Q},\vec{P},t)$ is expanded in a power series in Q_i, P_i, then the resulting series contains no linear terms if $(x^g, p_x^g, y_g, p_y^g, z_g, p_z^g)(t)$ is a solution of Hamilton's equations.

1.2 Numerical Integration

Consider a set of m first-order differential equations of the form

$$\dot{y}_i = f_i(y_1, \cdots, y_m; t), \qquad i = 1, \ldots m \tag{1.28}$$

or, in vector notation,

$$\dot{\vec{y}} = \vec{f}(\vec{y}; t). \tag{1.29}$$

Our goal is to solve these equations numerically with a certain accuracy, given some initial conditions. The equations could have been arrived at directly, *e.g.* from Hamilton's equations. Alternatively, they might be obtained by making appropriate substitutions in some other system of

equations that is not of first order. Consider, for example, the following second-order equations:

$$\begin{aligned} \ddot{q}_1 &= f_1(\vec{q}, \dot{\vec{q}}; t), \\ \ddot{q}_2 &= f_2(\vec{q}, \dot{\vec{q}}; t). \end{aligned} \tag{1.30}$$

Then we can write

$$\begin{aligned} y_1 &= q_1, \\ y_2 &= \dot{q}_1, \\ y_3 &= q_2, \\ y_4 &= \dot{q}_2, \end{aligned} \tag{1.31}$$

and we obtain the set of first-order equations,

$$\begin{aligned} \dot{y}_1 &= y_2, \\ \dot{y}_2 &= f_1(\vec{y}, \dot{\vec{y}}; t), \\ \dot{y}_3 &= y_4, \\ \dot{y}_4 &= f_2(\vec{y}, \dot{\vec{y}}; t). \end{aligned} \tag{1.32}$$

Now suppose we want to integrate the equations from t^{in} to t^{fin}. To do this, divide the time axis into N steps of length h, where

$$\begin{aligned} t^0 &= t^{\text{in}}, \\ t^1 &= t^{\text{in}} + h, \\ &\vdots \\ t^N &= t^{\text{in}} + Nh = t^{\text{fin}}. \end{aligned} \tag{1.33}$$

Our goal is to compute the vectors $\vec{y}^n = \vec{y}(t^n),\ (n = 1, \ldots, N)$, given initial conditions $\vec{y}^0$.

There are many numerical schemes for integrating ordinary differential equations. A key consideration is the accuracy of these schemes. We say that a method is an "m^{th} order method" if it is locally correct through order h^m, and makes local errors of order h^{m+1}. That is, for an m^{th} order numerical scheme,

$$\vec{y}^{n+1}_{\text{numerical}} = \vec{y}^n_{\text{exact}} + O(h^{m+1}). \tag{1.34}$$

The simplest numerical scheme, due to Euler, follows directly from Taylor's theorem,

$$\vec{y}^{n+1} = y^n + h\dot{y}^n + O(h^2) = y^n + hf^n + O(h^2). \tag{1.35}$$

The Euler method is a first order algorithm given by

$$\vec{y}^{n+1} = y^n + hf^n. \tag{1.36}$$

Note that, in the Euler scheme, to take one step we must evaluate the function f at just one point, $f^n = f(\vec{x}^n; t^n)$. More sophisticated schemes, such as the Runge-Kutta schemes, make use of derivatives of f at more than one point in the interval $[t^n, t^{n+1}]$. Other approaches, commonly associated with the name of Adams and others, make use of several values of $\vec{y}$ at previous time-steps to take a single step. Finally, symplectic integration schemes are generally the methods of choice for modeling Hamiltonian systems, especially the long-term behavior of Hamiltonian systems. All of these are discussed in the following sections.

1.3 Runge-Kutta Algorithms

As an example of a Runge-Kutta scheme, consider the following third order algorithm:

$$y^{n+1} = y^n + \frac{1}{6}(a + 4b + c), \tag{1.37}$$

where

$$\begin{aligned} a &= hf(y^n, t^n), \\ b &= hf(y^n + a/2, t^n + h/2), \\ c &= hf(y^n + 2b - a, t^n + h). \end{aligned} \tag{1.38}$$

Note that this scheme requires three function evaluations, namely at the beginning, middle, and end of the interval.

There are an infinite number of fourth-order schemes that differ with regard to the locations for function evaluations and the weights a, b, etc. A commonly used 4th-order algorithm is the following:

$$y^{n+1} = y^n + \frac{1}{6}(a + 2b + 2c + d), \tag{1.39}$$

where

$$\begin{aligned} a &= hf(y^n, t^n), \\ b &= hf(y^n + a/2, t^n + h/2), \\ c &= hf(y^n + b/2, t^n + h/2), \\ d &= hf(y^n + c, t^n + h). \end{aligned} \tag{1.40}$$

It is rare to see Runge-Kutta algorithms used beyond 6th or 7th order, since the number of function evaluations in higher-order schemes increases rapidly, and other methods, such as the Predictor-Corrector methods that follow, are much more efficient.

A program that performs 4th-order Runge-Kutta integration follows [2]. To use it, one must set the number of equations to be integrated (which is presently specified in `parameter` statements at the beginning of subroutines). The user must also rewrite `subroutine eval`, which evaluates the function $\vec{f}$ in the equations $\dot{\vec{y}} = \vec{f}(\vec{y}, t)$. As shown below, the code contains the four equations for the transverse dynamics of a particle in a constant magnetic field. The field strength is chosen so that the period of the oscillator is one.

- **Problem 1.6**
  Show that the Runge-Kutta scheme described by Eq. (1.37) and Eq. (1.38) is in fact accurate through third order. To do this, first write down the Taylor series expansion of y_{n+1} around the point y_n:
  $$y_{n+1} = y_n + h\dot{y}_n + \frac{h^2}{2}\ddot{y}_n + \frac{h^3}{6}y_n^{(3)} + O(h^4), \tag{1.41}$$
  and compute the derivative terms using the relation
  $$\frac{d}{dt} = \frac{\partial}{\partial t} + \dot{y}\frac{\partial}{\partial y} = \frac{\partial}{\partial t} + f\frac{\partial}{\partial y} \tag{1.42}$$
  Next substitute Eq. (1.38) into Eq. (1.37), and using Taylor's theorem again, obtain a series solution for y^{n+1}. Verify that this agrees with the first series you obtained.

```
      program rkexample
! Numerical integration of the trajectory of a particle in
! an idealized solenoid using 4th order Runge-Kutta
      implicit real(a-h,o-z)
      parameter(nx=4)
      dimension y(nx)
! integrate to tfin using nsteps time-steps
      write(6,*)'input tfin,nsteps'
      read(5,*)  tfin,nsteps
      h=tfin/nsteps
! initial conditions:
      y=(/1.0,0.,0.5,0./)
! perform the numerical integration:
      t=0.
      call prnt(t,y)
      call rk4(h,nsteps,t,y)
      stop
      end
```

Main Program for Runge-Kutta Example

```
      subroutine prnt(t,y)
! diagnostic routine
      implicit real(a-h,o-z)
      parameter(nx=4)
      dimension y(nx)
      write(16,10)t,y(1),y(2),y(3),y(4)
   10 format(5(1x,e14.7))
      return
      end
```

Diagnostic Routine for Runge-Kutta Example

```
      subroutine rk4(h,ns,t,y)
      implicit real(a-h,o-z)
      parameter(nx=4)
      dimension y(nx),yt(nx),f(nx),a(nx),b(nx),c(nx),d(nx)
      tint=t
      do 100 i=1,ns
        call eval(t,y,f)
        a=h*f
        yt=y+0.5*a
        tt=t+0.5*h
        call eval(tt,yt,f)
        b=h*f
        yt=y+0.5*b
        tt=t+0.5*h
        call eval(tt,yt,f)
        c=h*f
        yt=y+c
        tt=t+h
        call eval(tt,yt,f)
        d=h*f
        y=y+(a+2.0*b+2.0*c+d)/6.0
        t=tint+i*h
        call prnt(t,y)
  100 continue
      return
      end
!
      subroutine eval(t,y,f)
      implicit real(a-h,o-z)
      parameter(nx=4)
      dimension y(nx),f(nx)
      alfa=4.0*asin(1.0)
      a2=alfa**2
      f(1)=y(2)
      f(2)=-a2*y(1)
      f(3)=y(4)
```

```
      f(4)=-a2*y(3)
      return
      end
```

rk4 and eval Routines for Runge-Kutta Example

1.4 Adams Schemes

The Runge-Kutta schemes described previously are examples of "single-step" methods; they make use only of newly obtained information (such as several function evaluations in the interval h) to perform the next time-step. As one might imagine, it is very inefficient to do all those calculations required to perform a time step and then disregard that information when computing the next time-step. In contrast, multi-step methods make use of information at previous time steps. Since these methods basically approximate the trajectory by a polynomial (possibly of high order), it is inadvisable to attempt to take large time steps even though the algorithm may be of high order. Thus, these methods are best used when very high accuracy is desired. Here we will describe one such approach, a predictor-corrector scheme associated with the names Adams, Bashforth, and Moulton. Following Dragt [3], we will simply call these Adams methods. As an example, an Adams method that is locally accurate through order 11 uses $\vec{f}(\vec{y}^n, t^n)$, $\vec{f}(\vec{y}^{n-1}, t^{n-1})$,$\cdots$, $\vec{f}(\vec{y}^{n-10}, t^{n-10})$, to compute $\vec{y}^{n+1}$. A summary of the procedure is shown below:

Adams procedure with local accuracy h^M

1. Starting with y^0, use some procedure (e.g. a high-order Runge-Kutta with fractional time-step such as h/4) to compute (y^1, f^1),(y^2, f^2),. . .,(y^M, f^M).

2. Obtain y^{M+1} by performing PECEC, where P=predict y^{M+1}, E=evaluate f^{M+1}, C=correct y^{M+1}.

3. Update the table of f's to include f^{M+1}.

4. Discard the earliest values of y and f so that only the most recent M values remain.

5. Return to set 2 for the next time-step.

The Predictor/Corrector formulas are shown below:

$$y^{n+1} = y^n + h\sum_{k=0}^{M} b_k^M f^{n-k} \qquad (predictor) \tag{1.43}$$

$$y^{n+1} = y^n + h\sum_{k=0}^{M} a_k^M f^{n-k+1} \qquad (corrector) \tag{1.44}$$

The coefficients a_k^M and b_k^M can be found in the literature.

1.5 Symplectic Integration

Many of the differential equations of mathematical physics are symplectic in nature. As we will see later, Hamilton's equations define symplectic mappings. Symplectic integration algorithms are numerical algorithms that preserve the underlying symplectic nature of the equations to be integrated. The first 3rd-order symplectic integrator was developed by Ronald Ruth [4]; it was applicable to Hamiltonian systems of a particular form, namely $H = A(\vec{q}) + V(\vec{p})$. Later, Etienne Forest, Ruth, Fillipo Neri, and others, went on to develop more general 4th-order symplectic algorithms based on Lie methods [5]. Finally, Yoshida showed how, given an algorithm of order $2n$ (subject to certain conditions), one can generate an algorithm of order $2n+2$ [6]. The wide applicability of Yoshida's result was not fully appreciated until it was identified and exploited by Forest et al. [7].

There is not an *explicit* symplectic integration algorithm that works for arbitrary Hamiltonians. However, there are explicit methods for Hamiltonians that can be written as a sum of terms, each of which can be solved separately. Since any monomial of the phase space variables, $(x^i p_x^j y^k p_y^l)$ is itself integrable, it follows that any Hamiltonian that is a finite sum of monomials (as often occurs in magnetic optics) can be treated using these so-called *split-operator symplectic integration* techniques. In principle these can be extended to any order using

the method of Yoshida. There is also a 2nd order *implicit* algorithm that can be applied to *any* Hamiltonian, which can also be extended to high order using the method of Yoshida. All of these are discussed below.

- **Problem 1.7** (Paul Channell)
  Let $H = (x^i p_x^j y^k p_y^l)$. Solve Hamilton's equations for this system.

1.5.1 2nd Order Leap-Frog

The 2nd order leap-frog algorithm has been widely used in the computational plasma physics community. Consider the equations

$$\frac{dx}{dt} = v, \tag{1.45}$$

$$\frac{dv}{dt} = f(x,t). \tag{1.46}$$

The statement is usually made that "the positions, x^n, are known times, t^n, and the velocities, $v^{n+1/2}$ are known at half-times, $t^{n+1/2}$". Discretizing the above equations, we obtain

$$x^{n+1} - x^n = hv^{n+1/2}, \tag{1.47}$$

$$v^{n+1/2} - v^{n-1/2} = hf^n. \tag{1.48}$$

This leads to the well known leap-frog algorithm,

$$x^{n+1} = x^n + hv^{n+1/2}, \tag{1.49}$$

$$v^{n+1/2} = v^{n-1/2} + hf^n. \tag{1.50}$$

Given $(x^n, v^{n-1/2})$, one first uses Eq. (1.50) to obtain $v^{n+1/2}$, and then Eq. (1.49) to obtain x^{n+1}; this process is repeated for the desired number of steps. In the one-dimensional case, it turns out that a map is symplectic if and only if its Jacobian has determinant equal to one. It is easily demonstrated that this is the case for the above algorithm, i.e.

$$\det \left(\begin{array}{c|c} \frac{\partial x^{n+1}}{\partial x^n} & \frac{\partial x^{n+1}}{\partial v^{n-1/2}} \\ \hline \frac{\partial v^{n+1/2}}{\partial x^n} & \frac{\partial v^{n+1/2}}{\partial v^{n-1/2}} \end{array} \right) = 1. \tag{1.51}$$

- **Problem 1.8**
  Verify Eq. (1.51).

1.5.2 Split-Operator Symplectic Integration

Consider a Hamiltonian that can be written as a sum of two terms,

$$H = H_1 + H_2. \tag{1.52}$$

Suppose we can obtain the mapping $\mathcal{M}_1$ corresponding to H_1 and the mapping $\mathcal{M}_2$ corresponding to H_2. Then the following algorithm is accurate through 2nd order:

$$\mathcal{M}(\tau) = \mathcal{M}_1(\tau/2)\ \mathcal{M}_2(\tau)\ \mathcal{M}_1(\tau/2). \tag{1.53}$$

This approach is easily generalized to more splittings. For example, consider a Hamiltonian that can be written as a sum of three terms,

$$H = H_1 + H_2 + H_3. \tag{1.54}$$

Then a 2nd order algorithm is given by

$$\mathcal{M}(\tau) = \mathcal{M}_1(\tau/2)\ \mathcal{M}_2(\tau/2)\ \mathcal{M}_3(\tau)\ \mathcal{M}_2(\tau/2)\ \mathcal{M}_1(\tau/2). \tag{1.55}$$

Returning to the two-term case, Forest and Ruth showed that the following algorithm is accurate through 4th order:

$$\mathcal{M}(\tau) = \mathcal{M}_1(\frac{s}{2})\ \mathcal{M}_2(s)\ \mathcal{M}_1(\frac{\alpha s}{2})\ \mathcal{M}_2((\alpha-1)s)\ \mathcal{M}_1(\frac{\alpha s}{2})\ \mathcal{M}_2(s)\ \mathcal{M}_1(\frac{s}{2}), \tag{1.56}$$

where

$$\alpha = 1 - 2^{1/3}, \quad s = \tau/(1+\alpha). \tag{1.57}$$

In other words, this is a 4th-order algorithm that is a product of seven maps. Note that α is approximately equal to -0.26, and in particular α is negative. This means that this middle three steps in the seven-step procedure have negative time steps.

1.5.3 The Method of Yoshida

The main result due to Yoshida, as well as the wide applicability of Yoshida's approach, is described in Ref. [6]. Let $\mathcal{M}_{2n}$ denote a mapping

that is an approximate solution to a problem that is accurate through order $2n$. Also, suppose $\mathcal{M}_{2n}$ has the property that

$$\mathcal{M}_{2n}(\tau)\mathcal{M}_{2n}(-\tau) = I, \tag{1.58}$$

where I is the identity mapping. Then the following is accurate through order $2n+2$:

$$\mathcal{M}_{2n+2}(\tau) = \mathcal{M}_{2n}(z_0\tau)\ \mathcal{M}_{2n}(z_1\tau)\ \mathcal{M}_{2n}(z_0\tau) \tag{1.59}$$

where

$$z_0 = \frac{1}{2 - 2^{1/(2n+1)}}, \qquad z_1 = \frac{-2^{1/(2n+1)}}{2 - 2^{1/(2n+1)}} \tag{1.60}$$

- **Problem 1.9**
  Let $\mathcal{M}_2$ denote the map for the leap-frog algorithm, in the form of Eq. (1.53). Show that by following the method of Yoshida, the resulting 4th order algorithm is the algorithm of Forest and Ruth given in Eqs. (1.56) and (1.57).

- **Problem 1.10**
  For a system governed by a Hamiltonian H, consider the following approximation, which is due to Poincare:

$$q^f = q + \tau\frac{\partial H}{\partial x_2}(\frac{q+q^f}{2}, \frac{p+p^f}{2}), \tag{1.61}$$

$$p^f = p - \tau\frac{\partial H}{\partial x_1}(\frac{q+q^f}{2}, \frac{p+p^f}{2}). \tag{1.62}$$

  Here x_1 and x_2 refer to the arguments q and p, respectively. Prove that this approximation is accurate through second order, and that it satisfies the time reversal property of Eq. (1.58). It follows that, using the method of Yoshida, one can construct an arbitrary order implicit symplectic integrator for any Hamiltonian system. Furthermore, as is evident from the above formulas, the integrator involves only first derivatives of the Hamiltonian with respect to its arguments. See E. Forest *et al.*, Physics Letters A 158, p99 (1991).

- **Problem 1.11** (Paul Channell)
  Magnetic optics calculations are often performed by expanding the square root in the relativistic Hamiltonian, Eq. (1.11). However, consider the case of motion in a purely magnetostatic field. Then the Hamiltonian is given by

$$H = \sqrt{m^2c^4 + c^2(\vec{p} - q\vec{A})^2} \tag{1.63}$$

  Now define a new Hamiltonian, $\mathcal{H}$, according to

$$\mathcal{H} = \frac{H^2}{2}. \tag{1.64}$$

  Show that the geometry of the trajectories in H and $\mathcal{H}$ is identical, and that the solution of the equations of motion in the two systems is related by a scaling in time, namely $t \rightarrow t/E$, where E is the energy. Note: This makes it possible to symplectically integrate the equations of motion without computing a square root; this can have beneficial performance consequences in some applications. Also, if A is a polynomial in (x, y, z), then $\frac{H^2}{2}$ is a polynomial in (x, p_x, y, p_y, z, p_z), and the results of Problem 1.7 (on monomial Hamiltonians) can be combined with the abovementioned split-operator techniques to develop an arbitrary order, explicit symplectic integrator for particle motion (in time) in magnetostatic systems. The results of this problem are also applicable to systems where z is the independent variable and where A_z is zero, as can be seen from Eq. (1.20).

A program that performs 2nd order and 4th order symplectic integration follows. Three subroutines are shown: `symp24`, which is the driver routine, `map1` and `map2`, which perform the operations associated with $\mathcal{M}_1$ and $\mathcal{M}_2$, respectively. As before, the program, as shown, simulates the transverse dynamics of a particle in a constant magnetic field. As we will see in the following chapter, the Hamiltonian for this system is given by

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{\alpha^2}{2}(x^2 + y^2). \tag{1.65}$$

For the sake of illustration, it has been split as $H = H_1 + H_2$, where

$$H_1 = \frac{1}{2}(p_x^2 + p_y^2), \qquad H_2 = \frac{\alpha^2}{2}(x^2 + y^2). \tag{1.66}$$

The map $\mathcal{M}_1$ is given by

$$\begin{aligned} x^{fin} &= x^{in} + p_x^{in}\tau, & p_x^{fin} &= p_x^{in}, \\ y^{fin} &= y^{in} + p_y^{in}\tau, & p_y^{fin} &= p_y^{in}. \end{aligned} \tag{1.67}$$

The map $\mathcal{M}_2$ is given by

$$\begin{aligned} x^{fin} &= x^{in}, & p_x^{fin} &= p_x^{in} - \alpha^2 x^{in}\tau, \\ y^{fin} &= y^{in}, & p_y^{fin} &= p_y^{in} - \alpha^2 y^{in}\tau. \end{aligned} \tag{1.68}$$

- **Problem 1.12**
  Use Hamilton's equations to show that $\mathcal{M}_1$ and $\mathcal{M}_2$ correspond to (1.67) and (1.68).

```
      subroutine map1(tau,y,yt)
      implicit real(a-h,o-z)
      dimension y(*),yt(*)
      yt(1)=y(1)+tau*y(2)
      yt(2)=y(2)
      yt(3)=y(3)+tau*y(4)
      yt(4)=y(4)
      return
      end
!
      subroutine map2(tau,y,yt)
      implicit real(a-h,o-z)
      dimension y(*),yt(*)
      alfa=4.0*asin(1.0)
      a2=alfa**2
      yt(1)=y(1)
      yt(2)=y(2)-tau*a2*y(1)
      yt(3)=y(3)
      yt(4)=y(4)-tau*a2*y(3)
      return
      end
```

Routines map1 and map2 for Symplectic Integration Example

```
      subroutine symp24(h,ns,t,norder,y)
      implicit real(a-h,o-z)
      parameter(nx=4)
      dimension y(nx),yt(nx)
      tint=t
      alf=1.-2.**(1./3.)
      tau2=h/(1.+alf)
      tau1=0.5*tau2
      tau3=alf*tau1
      tau4=(alf-1.)*tau2
! use 2nd order symplectic if norder<=2, otherwise use 4th order
      do 100 i=1,ns
      if(norder.le.2)then
        call map1(0.5*h,y,yt)
        call map2(h,yt,y)
        call map1(0.5*h,y,yt)
      else
        call map1(tau1,y,yt)
        call map2(tau2,yt,y)
        call map1(tau3,y,yt)
        call map2(tau4,yt,y)
        call map1(tau3,y,yt)
        call map2(tau2,yt,y)
        call map1(tau1,y,yt)
      endif
      y=yt
      t=tint+i*h
      call prnt(t,y)
  100 continue
      return
      end
```

Driver Routine for Symplectic Integration Example

Chapter 2

Linear Magnetic Optics

2.1 Equations for the Linear Map

In this chapter we will deal with the analytical and numerical computation of linear transfer maps. Transfer map techniques provide a powerful framework in which to analyze and optimize beam transport systems. By analyzing and manipulating maps, instead of simply tracking single particle trajectories, one can design transport systems to have desired properties, such as the absence or minimization of certain nonlinear effects. Analytical representations of transfer maps are available for only a few idealized beamline elements, and, in particular, analytical results are not available for beamline elements with realistic fringe fields. As a result, we must often resort to computing maps numerically rather than using analytical formulas. But as we will see, even the numerical computation of maps is a relatively simple, straightforward operation that should not cause anxiety in most cases.

In accelerator physics one is usually interested in trajectories near some particular trajectory, referred to as the "design," "reference," "synchronous", or "fiducial" trajectory. We will usually call this as the "given" trajectory, denoted by a superscript "g", as in ζ^g. Occasionally we will also use the symbol "o," as in p^o, β_o, and γ_o.

We will start by dealing with systems for which it is natural to use z as the independent variable. As stated previously, the Hamiltonian for such a system is obtained by setting the original Hamiltonian,

$H(x, p_x, y, p_y, z, p_z; t)$, equal to $-p_t$, and solving for $-p_z$. As shown in Eq. (1.20), the new Hamiltonian, $K(x, p_x, y, p_y, t, p_t; z)$, is

$$K = -\left[(p_t + q\psi)^2/c^2 - m^2c^2 - (p_x - qA_x)^2 - (p_y - qA_y)^2\right]^{1/2} - qA_z. \tag{2.1}$$

In all that follows it will be convenient to work with dimensionless variables. Let

$$\bar{x} = x/l, \qquad \bar{p}_x = p_x/\delta \tag{2.2}$$

$$\bar{y} = y/l, \qquad \bar{p}_y = p_y/\delta \tag{2.3}$$

$$\bar{t} = \omega t, \qquad \bar{p}_t = p_t/(\omega l \delta) \tag{2.4}$$

where l, δ and ω are constants. The quantity l is a scale length, δ is a scale momentum, and ω is a scale frequency (i.e. $1/\omega$ is a scale time). For most problems we will set $l = 1$ m. The choices of δ and ω will depend on the situation. When treating magnetostatic elements, it is conventional to set δ equal to the design momentum, p^o, of the system under consideration. When dealing with acceleration by rf cavities, we cannot scale according to p^o, since the design momentum is not a constant; instead we set $\delta = mc$. In this case it is also useful to set ω equal to the frequency of the rf fields, or some multiple thereof. The transformation to dimensionless variables is canonical, and the new variables are governed by the following Hamiltonian, $K^{\rm new}$:

$$K^{\rm new}(\bar{x}, \bar{p}_x, \bar{y}, \bar{p}_y, \bar{t}, \bar{p}_t) = \tag{2.5}$$
$$-\tfrac{1}{l}\left[(\tfrac{\omega l}{c}\bar{p}_t + \tfrac{q}{\delta c}\psi)^2 - (\tfrac{mc}{\delta})^2 - (\bar{p}_x - \tfrac{q}{\delta}A_x)^2 - (\bar{p}_y - \tfrac{q}{\delta}A_y)^2\right]^{1/2} - \tfrac{q}{\delta l}A_z,$$

where

$$\vec{A} = \vec{A}(l\bar{x}, l\bar{y}, \bar{t}/\omega; z) \tag{2.6}$$

$$\psi = \psi(l\bar{x}, l\bar{y}, \bar{t}/\omega; z). \tag{2.7}$$

Lastly, go to the reference trajectory by setting

$$X = \bar{x} - \bar{x}^g, \qquad P_x = \bar{p}_x - \bar{p}_x^g \tag{2.8}$$

$$Y = \bar{y} - \bar{y}^g, \qquad P_y = \bar{p}_y - \bar{p}_y^g \tag{2.9}$$

$$T = \bar{t} - \bar{t}^g, \qquad P_t = \bar{p}_t - \bar{p}_t^g \tag{2.10}$$

This transformation is also canonical, so the deviation variables are also governed by a Hamiltonian, which we will denote H. The new Hamiltonian is

$$H(X, P_x, Y, P_y, T, P_t) = -\frac{q}{\delta l} A_z$$
$$-\frac{1}{l}\left[(\frac{\omega l}{c} P_t + \frac{\omega l}{c}\bar{p}_t^g + \frac{q}{\delta c}\psi)^2 - (\frac{mc}{\delta})^2 - (P_x + \bar{p}_x^g - \frac{q}{\delta}A_x)^2 - (P_y + \bar{p}_y^g - \frac{q}{\delta}A_y)^2\right]^{1/2}$$
$$-\frac{d\bar{x}^g}{dz}(P_x + \bar{p}_x^g) + \frac{d\bar{p}_x^g}{dz}X - \frac{d\bar{y}^g}{dz}(P_y + \bar{p}_y^g) + \frac{d\bar{p}_y^g}{dz}Y - \frac{d\bar{t}^g}{dz}(P_t + \bar{p}_t^g) + \frac{d\bar{p}_t^g}{dz}T \quad (2.11)$$

where

$$\vec{A} = \vec{A}(lX + l\bar{x}^g, lY + l\bar{y}^g, (T + \bar{t}^g)/\omega; z) \quad (2.12)$$
$$\psi = \psi(lX + l\bar{x}^g, lY + l\bar{y}^g, (T + \bar{t}^g)/\omega; z). \quad (2.13)$$

(Often many terms in Eq. (2.11) will be zero, as would be the case, for example, if $x^g = p_x^g = y_g = p_y^g = 0$). At this stage we expand H around the given trajectory, $X = P_x = Y = P_y = T = P_t = 0$. By construction it will turn out that all the linear terms vanish, as demostrated in Problem 1.5. Also, we can drop any term that is a constant or just a function of z, since such terms do not affect the resulting equations of motion. Thus, we obtain

$$H = H_2 + H_3 + H_4 + \cdots, \quad (2.14)$$

where each H_n is a homogeneous polynomial of degree n in (X, P_x, Y, P_y, T, P_t). The linear dynamics are governed by H_2, and the quantities H_2 through H_n determine the dynamics through order $n - 1$.

It can be shown that the linear transfer map, M, obeys the differential equation

$$\frac{dM}{dt} = JSM, \quad (2.15)$$

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

$$H_2 = \frac{1}{2}\sum_{a,b=1}^{2m} S_{ab}\zeta_a\zeta_b. \quad (2.16)$$

and where ζ denotes the collection of canonical coordinates and momenta. For example, in one dimension, with $\zeta = (x, p_x)$, if $H =$

$\frac{1}{2}ax^2 + bxp_x + \frac{1}{2}cp_x^2$, then

$$S = \begin{pmatrix} a & b \\ b & c \end{pmatrix}. \tag{2.17}$$

In Eq. (2.15), the precise form of the matrix J depends on the ordering of the variables in the definition of ζ. For example, if we set $\zeta = (X, P_x, Y, P_y, T, P_t)$, then J is a matrix that has copies of a 2x2 matrix J_2 on the diagonal and zeros elsewhere, with

$$J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{2.18}$$

So, for example, in three dimensions,

$$J = \left(\begin{array}{cc|cc|cc} 0 & 1 & & & & \\ -1 & 0 & & & & \\ \hline & & 0 & 1 & & \\ & & -1 & 0 & & \\ \hline & & & & 0 & 1 \\ & & & & -1 & 0 \end{array}\right). \tag{2.19}$$

If, instead, we had set $\zeta = (X, Y, T, P_x, P_y, P_t)$, then J would be of the form

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{2.20}$$

where I is the 3x3 identity matrix. In all the follows we will use the ordering in which the positions and momenta are interleaved, i.e. $\zeta = (X, P_x, Y, P_y, T, P_t)$.

In closing we note that Eq. (2.15) provides a means to compute linear transfer maps even in the presence of fringe fields. All that is required is a knowledge of the electromagnetic potentials, and the ability to integrate (at most 36) ordinary differential equations. It is also worth commenting that, given a linear, time dependent dynamical system, and a need to determine final conditions from initial conditions, it is highly inefficient to integrate the trajectories. For example, given 1,000,000 initial conditions, it would be extremely time consuming to perform numerical integration on *all* these trajectories, when you could

obtain the same results by integrating a small number of equations (for the map) and obtain the final conditions through 1,000,000 matrix multiplications. (An exception to this rule is the case in which the (presumably linear) forces depend on the phase space variables $\zeta(t)$; but in this case the problem is not really linear. Another exception to this rule is the case in which the system has a very large number of degrees of freedom, since the resulting matrix would be enormous.) Finally, note that the concept of calculating maps instead of naively calculating trajectories applies to nonlinear systems as well, as will be discussed in Chapter 3 on Lie Methods. But for the remainder of this chapter, we will concentrate linear dynamical systems.

2.2 Rectilinear Magnetostatic Elements

For magnetic multipoles excluding bending magnets (i.e. for magnetic quadrupoles, sextupoles, octupoles, etc.), as well as the drift space, we will assume that the design trajectory is along the z-axis of a Cartesian coordinate system:

$$\bar{x}^g = \bar{p}_x^g = \bar{y}^g = \bar{p}_y^g = 0. \tag{2.21}$$

The temporal variables satisfy

$$t^g = \frac{z}{v^o}, \tag{2.22}$$

$$p_t^g = constant, \tag{2.23}$$

where $v^o \equiv v^g$ is the velocity on the design trajectory, $\beta^o = v^o/c$, and $\gamma^o = 1/\sqrt{1-(\beta^o)^2}$. For these elements we will choose

$$\delta = p^o, \tag{2.24}$$

$$\omega l/c = 1 \ (\Rightarrow \omega = c/l), \tag{2.25}$$

$$l = 1 \text{ m}, \tag{2.26}$$

where p^o is the design momentum. Recall that p_t is the negative of the total energy, $p_t = -(\gamma mc^2 + q\psi)$. Assuming ψ equals zero on the reference trajectory (in fact, it can be chosen to be identically zero for magnetostatic elements), it follows that $p_t^g = -\gamma mc^2$. But in dimensionless variables, this quantity is scaled by $\omega l\delta$ (see Eq. (2.4)). This

leads to the surprising result that, though p_t^g is proportional to $-\gamma^o$, the dimensionless variable $\bar{p}_t^g$ is given by

$$\bar{p}_t^g = -\frac{1}{\beta^o}. \tag{2.27}$$

In what follows (see, for example, Eq. (2.29), we will expand a square root that contains the terms $(p_t^g)^2 - 1/(\gamma^o\beta^o)^2$. Thanks to Eq. (2.27), this equals one:

$$(p_t^g)^2 - \frac{1}{(\gamma^o\beta^o)^2} = 1. \tag{2.28}$$

- **Problem 2.1**
  Verify Eq. (2.27) and Eq. (2.28).

Note Well: From now on we will cease using the notation (X, P_x, Y, P_y, T, P_t), and instead use (x, p_x, y, p_y, t, p_t) to denote **dimensionless deviations from the given trajectory**.

2.2.1 Drift Space

In this case the Hamiltonian given in Eq. (2.11) reduces to

$$H = -\sqrt{(p_t - \frac{1}{\beta_o})^2 - \frac{1}{(\gamma^o\beta^o)^2} - p_x^2 - p_y^2} - \frac{1}{\beta^o}p_t. \tag{2.29}$$

Expanding the Hamiltonian, we obtain $H = H_2 + H_3 + H_4 + \ldots$, where

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2\gamma_o^2\beta_o^2}p_t^2 \tag{2.30}$$

$$H_3 = -\frac{1}{2\beta_o}(p_x^2 + p_y^2)p_t + \frac{1}{2\gamma_o^2\beta_o^2}p_t^3 \tag{2.31}$$

$$H_4 = \frac{1}{8}(p_x^2 + p_y^2)^2 + \frac{1}{4}(\frac{3}{\beta_o^2} - 1)(p_x^2 + p_y^2)p_t^2 + \frac{1}{8\gamma_o^2\beta_o^2}(\frac{5}{\beta_o^2} - 1)p_t^4 \tag{2.32}$$

The mapping corresponding to H_2 is obviously

$$\begin{aligned} x^{fin} &= x^{in} + p_x^{in}z, & p_x^{fin} &= p_x^{in}, \\ y^{fin} &= y^{in} + p_y^{in}z, & p_y^{fin} &= p_y^{in}, \\ t^{fin} &= t^{in} + \frac{p_t^{in}}{\gamma_o^2\beta_o^2}z, & p_t^{fin} &= p_t^{in}. \end{aligned} \tag{2.33}$$

In matrix notation, the linear map is given by

$$M = \left(\begin{array}{cc|cc|cc} 1 & z & & & & \\ 0 & 1 & & & & \\ \hline & & 1 & z & & \\ & & 0 & 1 & & \\ \hline & & & & 1 & \frac{1}{\gamma_o^2\beta_o^2}z \\ & & & & 0 & 1 \end{array}\right). \tag{2.34}$$

Before leaving the treatment of the drift space, we emphasize that, due to the presence of the square root in Eq. (2.29), the drift is a *nonlinear* element. We can compute the exact, nonlinear map corresponding to Eq. (2.29) by solving Hamilton's equations. This is easy, since the Hamiltonian contains only momenta and not coordinates. The result is:

$$\begin{aligned} x^{fin} &= x^{in} + \frac{p_x^{in} z}{\sqrt{(p_t^{in} - \frac{1}{\beta_o})^2 - \frac{1}{(\gamma^o\beta^o)^2} - (p_x^{in})^2 - (p_y^{in})^2}}, \\ p_x^{fin} &= p_x^{in}, \\ y^{fin} &= y^{in} + \frac{p_y^{in} z}{\sqrt{(p_t^{in} - \frac{1}{\beta_o})^2 - \frac{1}{(\gamma^o\beta^o)^2} - (p_x^{in})^2 - (p_y^{in})^2}}, \\ p_y^{fin} &= p_y^{in}, \\ t^{fin} &= t^{in} - z\left[\frac{1}{\beta_o} + \frac{(p_t^{in} - 1/\beta_o)}{\sqrt{(p_t^{in} - \frac{1}{\beta_o})^2 - \frac{1}{(\gamma^o\beta^o)^2} - (p_x^{in})^2 - (p_y^{in})^2}}\right], \\ p_t^{fin} &= p_t^{in}. \end{aligned} \tag{2.35}$$

- **Problem 2.2**
  Verify that Eq. (2.35) is the solution of Hamilton's equations with Hamiltonian (2.29).

2.2.2 Magnetic Quadrupole

Consider a magnetic quadrupole oriented along the z-axis of a Cartesian coordinate system. In this case, the vector and scalar potentials can be

represented by

$$\begin{aligned} A_x(x,y,z) &= \frac{1}{4}g'(z)(x^3 - xy^2) + \cdots, \\ A_y(x,y,z) &= \frac{1}{4}g'(z)(x^2y - y^3) + \cdots, \\ A_z(x,y,z) &= \frac{1}{2}g(z)(y^2 - x^2) - \frac{1}{12}g''(z)(y^4 - x^4) + \cdots, \end{aligned} \tag{2.36}$$

$$\psi = 0, \tag{2.37}$$

where $g(z)$ denotes the quadrupole gradient (in Tesla/meter, for example), and where a prime denotes d/dz. Taking the curl of $\vec{A}$ gives

$$\begin{aligned} B_x(x,y,z) &= gy - \frac{1}{12}g''(y^3 + 3x^2y) + \cdots, \\ B_y(x,y,z) &= gx - \frac{1}{12}g''(x^3 + 3y^2x) + \cdots, \\ B_z(x,y,z) &= g'xy + \cdots \end{aligned} \tag{2.38}$$

Expanding the Hamiltonian, we obtain $H = H_2 + H_3 + H_4 + \ldots$, where

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}k(z)(x^2 - y^2) + \frac{1}{2\gamma_o^2\beta_o^2}p_t^2 \tag{2.39}$$

$$H_3 = -\frac{1}{2\beta_o}(p_x^2 + p_y^2)p_t + \frac{1}{2\gamma_o^2\beta_o^2}p_t^3 \tag{2.40}$$

$$\begin{aligned} H_4 = \tfrac{1}{12}k''(y^4 - x^4) - \tfrac{1}{4}k'\left[(x^3 - xy^2)p_x + (x^2y - y^3)p_y\right] + \tfrac{1}{8}(p_x^2 + p_y^2)^2 \\ + \tfrac{1}{4}(\tfrac{3}{\beta_o^2} - 1)(p_x^2 + p_y^2)p_t^2 + \tfrac{1}{8\gamma_o^2\beta_o^2}(\tfrac{5}{\beta_o^2} - 1)p_t^4 \end{aligned} \tag{2.41}$$

where the focusing strength, $k(z)$, is related to the quadrupole gradient according to

$$k(z) = \frac{q}{p^o}g(z). \tag{2.42}$$

Note that this is sometimes written

$$k(z) = g(z)/B\rho, \tag{2.43}$$

where $B\rho$ is the so-called magnetic rigidity of the reference particle,

$$B\rho \equiv \frac{p^o}{q}. \tag{2.44}$$

Now we will restrict ourselves to the linear map, which is governed by H_2. In this case, only the leading order term in A_z is required. (This should be evident from Eq. (2.11) and Eq. (2.36), since the leading term in A_z is quadratic, and this is the term that appears outside the square root in Eq. (2.11); in contrast, A_x and A_y contain only third order and higher order terms, which will result in third order and higher order terms in the Hamiltonian when Eq. (2.11) is expanded around the given trajectory.) It is easy to show that, for $g =$ constant, the matrix M is given by

$$M = \left(\begin{array}{cc|cc|cc} \cos\sqrt{k}z & \frac{1}{\sqrt{k}}\sin\sqrt{k}z & & & & \\ -\sqrt{k}\sin kz & \cos\sqrt{k}z & & & & \\ \hline & & \cosh\sqrt{k}z & \frac{1}{\sqrt{k}}\sinh\sqrt{k}z & & \\ & & \sqrt{k}\sinh\sqrt{k}z & \cosh\sqrt{k}z & & \\ \hline & & & & 1 & \frac{1}{\gamma_o^2\beta_o^2}z \\ & & & & 0 & 1 \end{array}\right). \tag{2.45}$$

- **Problem 2.3**
  The linear map for a magnetic quadrupole is of the form

$$M = \left(\begin{array}{cc|cc|cc} a_x & b_x & & & & \\ c_x & d_x & & & & \\ \hline & & a_y & b_y & & \\ & & c_y & d_y & & \\ \hline & & & & 1 & \frac{1}{\gamma_o^2\beta_o^2}z \\ & & & & 0 & 1 \end{array}\right). \tag{2.46}$$

  Find the differential equations for $a_x, b_x, c_x, d_x, a_y, b_y, c_y, d_y$. These are the equations that have to be solved numerically to treat quadrupole fringe fields. Show that, for $g =$ *constant*, this leads to Eq. (2.45).

2.2.3 Magnetic Solenoid

Consider a magnetic solenoid oriented along the z-axis of a Cartesian coordinate system. In this case, the vector and scalar potentials can be represented by

$$\begin{aligned} A_x(x,y,z) &= -\frac{B_o}{2}y + \frac{B_o''}{16}r^2 y + \cdots, \\ A_y(x,y,z) &= \frac{B_o}{2}x - \frac{B_o''}{16}r^2 x + \cdots, \\ A_z(x,y,z) &= 0, \qquad (2.47) \\ \psi &= 0, \qquad (2.48) \end{aligned}$$

where $B_o = B_z(r=0,z)$ is the longitudinal magnetic field on axis, and where a prime denotes d/dz. Taking the curl of $\vec{A}$ gives

$$\begin{aligned} B_x(x,y,z) &= -\frac{B_o'}{2}x + \frac{B_o'''}{16}xr^2 + \cdots, \\ B_y(x,y,z) &= -\frac{B_o'}{2}y + \frac{B_o'''}{16}yr^2 + \cdots, \\ B_z(x,y,z) &= B_o - \frac{B_o''}{4}r^2 + \cdots \qquad (2.49) \end{aligned}$$

Expanding the Hamiltonian, we obtain $H = H_2 + H_3 + H_4 + \ldots$, where

$$H_2 = \frac{1}{2}p^2 + \frac{\alpha^2}{2}r^2 - \alpha J_z + \frac{p_t^2}{2\gamma_o^2\beta_o^2} \qquad (2.50)$$

$$H_3 = (H_2/\beta_o)p_t \qquad (2.51)$$

$$\begin{aligned} H_4 = {} & \tfrac{1}{8}(p^2)^2 + \tfrac{\alpha^4 - \alpha\alpha''}{8}(r^2)^2 + \tfrac{3}{4}\alpha^2 r^2 p^2 - \tfrac{\alpha^2}{2}(\vec{r}\cdot\vec{p})^2 + \tfrac{\alpha'' - 4\alpha^3}{8}r^2 J_z \\ & -\tfrac{\alpha}{2}p^2 J_z + \tfrac{1-3/\beta_o^2)}{4}(2\alpha J_z - \alpha^2 r^2 - p^2)p_t^2 - \tfrac{1-5/\beta_o^2)}{8\beta_o^2\gamma_o^2}p_t^4 \qquad (2.52) \end{aligned}$$

where

$$\begin{aligned} r^2 &= x^2 + y^2 \\ p^2 &= p_x^2 + p_y^2 \\ J_z &= xp_y - yp_x \qquad (2.53) \end{aligned}$$

and where

$$\alpha(z) = \frac{1}{2}\frac{B_o}{B\rho}. \tag{2.54}$$

Now consider the linear map. We will write $H_2 = H_2^{foc} + H_2^{rot}$, where

$$\begin{aligned} H_2^{foc} &= \frac{1}{2}p^2 + \frac{\alpha^2}{2}r^2 + \frac{p_t^2}{2\gamma_o^2\beta_o^2} \\ H_2^{rot} &= -\alpha J_z \end{aligned} \tag{2.55}$$

The quantity H_2^{foc} causes transverse focusing (and it also contains the temporal drift-like term); H_2^{rot} simply causes rotations in the $x-y$ plane. Since J_z commutes with r^2 and p^2 (i.e. their Poisson bracket is zero, as will be covered in the next Chapter), M can be written as the product of two matrices, one corresponding to H_2^{foc} and one corresponding to H_2^{rot}. That is,

$$M = M^0 R, \tag{2.56}$$

where M^0 and R are of the form

$$M^0 = \left(\begin{array}{cc|cc|cc} a & b & & & & \\ c & d & & & & \\ \hline & & a & b & & \\ & & c & d & & \\ \hline & & & & 1 & \frac{1}{\gamma_o^2\beta_o^2}z \\ & & & & 0 & 1 \end{array}\right), \qquad R = \left(\begin{array}{cc|cc|cc} e & 0 & f & 0 & & \\ 0 & e & 0 & f & & \\ \hline g & 0 & h & 0 & & \\ 0 & g & 0 & h & & \\ \hline & & & & 1 & 0 \\ & & & & 0 & 1 \end{array}\right) \tag{2.57}$$

It is easy to show that, for $\alpha =$ constant, these matrices are given by

$$M^0 = \left(\begin{array}{cc|cc|cc} \cos\alpha z & \frac{1}{\alpha}\sin\alpha z & & & & \\ -\alpha\sin\alpha z & \cos\alpha z & & & & \\ \hline & & \cos\alpha z & \frac{1}{\alpha}\sin\alpha z & & \\ & & -\alpha\sin\alpha z & \cos\alpha z & & \\ \hline & & & & 1 & \frac{1}{\gamma_o^2\beta_o^2}z \\ & & & & 0 & 1 \end{array}\right) \tag{2.58}$$

$$R = \left(\begin{array}{cc|cc|cc} \cos\theta & 0 & \sin\theta & 0 & & \\ 0 & \cos\theta & 0 & \sin\theta & & \\ \hline -\sin\theta & 0 & \cos\theta & 0 & & \\ 0 & -\sin\theta & 0 & \cos\theta & & \\ \hline & & & & 1 & 0 \\ & & & & 0 & 1 \end{array}\right) \tag{2.59}$$

where $\theta = \alpha z$.

- **Problem 2.4**
  Find the differential equations for a, b, c, d and e, f, g, h in Eq. (2.57). Show that, for $\alpha =$ constant, these yield the matrices for the ideal solenoid, Eq.s (2.58) and (2.59).

2.3 Bending Magnets

The fact that accelerators are made up of physically separated beamline elements, each with their own linear and nonlinear fields, alignment errors, mispowering errors, etc., has lead to these begin described as "hopelessly complicated" Hamiltonian systems [8]. This is especially relevant to the analysis of circular machines. Rather than performing global analysis on such a Hamiltonian, the following approach is taken: One first computes the maps for individual beamline elements using a local coordinate system that is appropriate to the element. Then the maps are combined to produce a one-turn map, and global analysis is performed on that map.

So far we have dealt only with beamline elements for which the reference trajectory is a straight line. If all the elements are aligned on the reference axis, the situation is particularly simple since all the elements have the same local coordinate system, and no special effort is required to "sew" them together. The situation is markedly different for systems with bending magnets. The local coordinate patch for, say, a parallel-faced bend, and the elements that precede and follow it, are not coincident. They must be sewn together with mappings that connect the coordinate systems. A detailed discussion of this issue can be found in [9]. For the purpose of these lecture notes, we will now deal with the simplest kind of bending magnet, the ideal sector bend.

2.3.1 Ideal Sector Bend

An ideal sector bend is a bend for which particles enter and exit normal to the pole faces, and the pole faces subtend a nonzero angle. (The case of the pole faces being parallel to one another is the parallel-faced bend.) Unlike the elements that we have dealt with previously, the sector bend is treated in cylindrical coordinates. The starting point for our analysis is the single particle Hamiltonian in cylindrical coordinates, Eq(1.21),

$$K(r,p_r,z,p_z,t,p_t;\theta) = -r\left[(p_t+q\psi)^2/c^2 - m^2c^2 - (p_r-qA_r)^2 - (p_z-qA_z)^2\right]^{1/2} - qrA_\theta. \tag{2.60}$$

As before, we define dimensionless variables,

$$\bar{r} = r/l, \qquad \bar{p}_r = p_r/\delta \tag{2.61}$$

$$\bar{z} = z/l, \qquad \bar{p}_z = p_z/\delta \tag{2.62}$$

$$\bar{t} = \omega t, \qquad \bar{p}_t = p_t/(\omega l\delta) \tag{2.63}$$

As for the other magnetostatic elements, we will take $\delta = p^o$ and $\omega l/c = 1$, and $l = 1$ m. For the ideal sector bend, only A_θ is nonzero,

$$A_\theta = -\frac{r}{2}B_o, \tag{2.64}$$

which produces a uniform magnetic field of magnitude B_o in the z-direction.

- **Problem 2.5**
  Show that, if $\vec{A} = A_\theta\ \hat{\theta}$, as given in Eq. (2.64), the resulting magnetic field is given by $\vec{B} = \nabla \times \vec{A} = B_o\hat{z}$.

With this vector potential, the Hamiltonian in dimensionless variables is given by

$$K(\bar{r},\bar{p}_r,\bar{z},\bar{p}_z,\bar{t},\bar{p}_t;\theta) = -\bar{r}\sqrt{\bar{p}_t^2 - \frac{1}{(\gamma_o\beta_o)^2} - p_o^2(\bar{p}_r^2+\bar{p}_z^2)} + b_o\frac{\bar{r}^2}{2}, \tag{2.65}$$

where

$$b_o = \frac{q}{p^o}B_o. \tag{2.66}$$

Suppose the sector bend is placed at radius r_c in a ring. In the ideal case this will also be the radius of the reference particle, $1/b_o$.

- **Problem 2.6**
  Show that, given the Hamiltonian (2.65), a particle moving at constant radius with $r' = p_r' = 0$ has radial position $r = 1/b_o$.

Lastly, we define dimensionless deviations,

$$R = \bar{r} - \bar{r}_c, \qquad P_r = \bar{p}_r \tag{2.67}$$

$$Z = \bar{z}, \qquad P_z = \bar{p}_z \tag{2.68}$$

$$T = \bar{t} - \bar{t}^g, \qquad P_t = \bar{p}_t - \bar{p}_t^g \tag{2.69}$$

where, as before, $\bar{p}_t^g = -1/\beta_o$, and where $\bar{t}^g = \theta/(b_o r_c)$. The new Hamiltonian is given by

$$K = -r_c(1+\frac{R}{r_c})\sqrt{1 - 2P_t/\beta_o + P_t^2 - (P_r^2 + P_z^2)} + r_c\left[b_o R + \frac{b_o}{2r_c}R^2 - \frac{1}{b_o r_c \beta_o}P_t\right] \tag{2.70}$$

The notation commonly used for the transverse variables is to set $x = R$ and $y = Z$, where x denotes a horizontal deviation from r_c and y denotes a vertical deviation from the magnet midplane. We will use the notation (p_x, p_y) to denote (P_r, P_z). Also, we will write $\tau = -T$ and $\delta = -P_t$. Lastly, rather than using the angle θ, we use the arc length $s = r_c\theta$ as the independent variable. Putting it all together, we obtain

$$K(x, p_x, y, p_y, \tau, \delta; s) = -(1+\frac{x}{r_c})\sqrt{1 + 2\delta/\beta_o + \delta^2 - p_x^2 - p_y^2} + b_o x + \frac{b_o}{2r_c}x^2 + \frac{1}{b_o r_c \beta_o}\delta. \tag{2.71}$$

Expanding through second order, the linear map is governed by

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2 + \frac{\delta^2}{\gamma_o^2\beta_o^2}) + \frac{b_o}{2r_c}x^2 - \frac{x\delta}{\beta_o r_c} + x(b_o - \frac{1}{r_c}) - \frac{\delta}{\beta_o}(1 - \frac{1}{b_o r_c}). \tag{2.72}$$

Now consider the case where r_c is a fiducial trajectory, i.e. $r_c = 1/b_o$. Then the two linear terms vanish (by construction), and we obtain

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2 + \frac{\delta^2}{\gamma_o^2\beta_o^2}) + \frac{b_o^2}{2}x^2 - \frac{x\delta}{\beta_o r_c}. \tag{2.73}$$

The corresponding linear map is given by

$$M = \begin{pmatrix} \cos\theta & r_c \sin\theta & 0 & 0 & 0 & -\frac{r_c}{\beta_o}(1-\cos\theta) \\ -\frac{1}{r_c}\sin\theta & \cos\theta & 0 & 0 & 0 & -\frac{1}{\beta_o}\sin\theta \\ 0 & 0 & 1 & r_c\theta & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ \frac{1}{\beta_o}\sin\theta & \frac{r_c}{\beta_o}(1-\cos\theta) & 0 & 0 & 1 & -r_c\theta + \frac{r_c}{\beta_o^2}\sin\theta \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.74}$$

2.4 Accelerating Gap

Most ion linac codes treat beam dynamics in a gap using integrals that assume some effective beam velocity within the gap. Though such codes have been highly successful in the past, the goal of performing more accurate simulations provides impetus for using the correct linear map. Also, doing so provides an independent check on the accuracy of results based on the usual techniques. Besides, there is nothing exceptionally difficult about computing the linear map for an rf gap: there are z-dependent fields, just as was the case for a quadrupole with fringe fields; the only additional complication is that we have to numerically compute the design trajectory. This will also be the case in the treatment of bending magnets with fringe fields.

The vector potential associated with an rf gap can be expressed as

$$\begin{aligned} A_x &= \frac{e'(z)}{2\omega_\alpha} x \sin(\omega_\alpha t + \theta) \\ A_y &= \frac{e'(z)}{2\omega_\alpha} y \sin(\omega_\alpha t + \theta) \\ A_z &= -\frac{1}{\omega_\alpha}\{e(z) - \frac{r^2}{4}[e''(z) + \frac{\omega_\alpha^2}{c^2}e(z)]\}\sin(\omega_\alpha t + \theta), \end{aligned} \tag{2.75}$$

where $e(z)$ denotes the spatial part of the electric field at $r = 0$,

$$E_z(r=0) = e(z)\cos(\omega_\alpha t + \theta), \tag{2.76}$$

and where a prime denotes d/dz. For this example we will also allow for the possibility of magnetic quadrupole fields in addition to the gap

fields by including terms of the form in Eq. (2.36). The equations of motion for the design trajectory are given by

$$t_o' = \frac{-p_{to}/c}{\sqrt{p_{to}^2 - m^2c^4}}, \tag{2.77}$$

$$p_{to}' = -qe(z)\cos(\omega_\alpha t_o + \theta). \tag{2.78}$$

When treating and rf gap, it is natural to use different scaling parameters than those used previously for magnetostatic elements. In particular, we will take

$$\begin{aligned} \delta &= mc, \\ n\omega &= \omega_\alpha \\ l &= c/w. \end{aligned} \tag{2.79}$$

The Hamiltonian given in Eq. (2.11), expanded through second order, yields

$$H = H_{xy} + H_\phi, \tag{2.80}$$

where

$$\begin{aligned} H_{xy} = &\tfrac{\delta}{2lp_o}(\bar{p}_x^2 + \bar{p}_y^2) + \tfrac{qlg_m}{2\delta}(\bar{x}^2 - \bar{y}^2) - \tfrac{qe'\sin\phi_s}{2p_o\omega_\alpha}(\bar{x}\bar{p}_x + \bar{y}\bar{p}_y) \\ &+ \tfrac{l}{2\delta}[\tfrac{1}{p_o}(\tfrac{q}{2\omega_\alpha}e'\sin\phi_s)^2 - \tfrac{q}{2\omega_\alpha}(e'' + \tfrac{\omega_\alpha^2}{c^2}e)\sin\phi_s](\bar{x}^2 + \bar{y}^2) \end{aligned} \tag{2.81}$$

$$H_\phi = \frac{m^2\omega^2 l\delta}{2p_o^3}\bar{p}_t^2 - \frac{\omega_\alpha qe\sin\phi_s}{2\omega^2 l\delta}\bar{t}^2 \tag{2.82}$$

where we have used the notation $g_m(z)$ to denote the magnetic quadrupole gradient, and where the synchronous phase, ϕ_s, is given by $\phi_s = \omega_\alpha t_o(z) + \theta$.

In principle the linear map for an rf gap can be obtained from this Hamiltonian. However, it appears to require not only $e(z)$ but also its first two derivatives. In fact all that is required is $e(z)$ and its first derivative $e'(z)$. To see this we will transform the Hamiltonian by the following generating function,

$$F_3 = -\tilde{x}^2\frac{\Delta}{2} - \tilde{x}\bar{p}_x u^{-1/2} - \tilde{y}^2\frac{\Delta}{2} - \tilde{y}\bar{p}_y u^{-1/2} - \tilde{\phi}^2\frac{3l}{4}\frac{w'}{w} - \tilde{\phi}\bar{p}_\phi w^{-3/2}, \tag{2.83}$$

where

$$u = \frac{p_o}{\delta}, \tag{2.84}$$

$$w = \frac{p_o}{(m^2\omega^2 l^2 \delta)^{1/3}}, \tag{2.85}$$

and where Δ is given by

$$\Delta = \frac{l}{2}\Big[\frac{(\beta_o\gamma_o)'}{\beta_o\gamma_o} - \frac{(q/mc^2)e'\sin\phi_s}{\beta_o\gamma_o\omega_\alpha/c}\Big], \tag{2.86}$$

Note that since we have chosen $\delta = mc$ and $\omega l = c$ it follows that

$$u = w = \gamma_o\beta_o. \tag{2.87}$$

Following the usual procedure [1] the new variables $(\tilde{x}, \tilde{p}_x, \tilde{y}, \tilde{p}_y, \tilde{\phi}, \tilde{p}_\phi, z)$ are related to the original variables $(\bar{x}, \bar{p}_x, \bar{y}, \bar{p}_y, \bar{\phi}, \bar{p}_\phi, z)$ by the following relations:

$$\tilde{x} = u^{1/2}\bar{x}, \qquad \tilde{p}_x = \Delta u^{1/2}\bar{x} + u^{-1/2}\bar{p}_x, \tag{2.88}$$

$$\tilde{y} = u^{1/2}\bar{y}, \qquad \tilde{p}_y = \Delta u^{1/2}\bar{y} + u^{-1/2}\bar{p}_y, \tag{2.89}$$

$$\tilde{\phi} = u^{3/2}\bar{\phi}, \qquad \tilde{p}_\phi = \frac{3l}{2}(\frac{u'}{u})u^{3/2}\bar{\phi} + u^{-3/2}\bar{p}_\phi. \tag{2.90}$$

It follows that the new Hamiltonian is given by

$$H^{new} = H_x + H_y + H_\phi, \tag{2.91}$$

where

$$\begin{aligned} H_x = &\quad \frac{1}{2l}\tilde{p}_x^2 + \frac{l\Omega_x}{2}\tilde{x}^2 + \frac{qlg_m}{2p_o}\tilde{x}^2, \\ H_y = &\quad \frac{1}{2l}\tilde{p}_y^2 + \frac{l\Omega_y}{2}\tilde{y}^2 - \frac{qlg_m}{2p_o}\tilde{y}^2, \\ H_\phi = &\quad \frac{\tilde{p}_\phi^2}{2l} + \frac{l\Omega_\phi}{2}\tilde{\phi}^2, \end{aligned} \tag{2.92}$$

and where Ω_x, Ω_y, and Ω_ϕ are given by

$$\Omega_x = \Omega_y = \frac{(q/mc^2)(\omega_\alpha/c)}{2\beta_o^3\gamma_o^3}e\sin\phi_s + \frac{1}{2}(1+\frac{\gamma_o^2}{2})\Big(\frac{(q/mc^2)e\cos\phi_s}{\beta_o^2\gamma_o^2}\Big)^2, \tag{2.93}$$

$$\Omega_\phi = \frac{(\beta_o^2+\frac{1}{2})}{\beta_o^3\gamma_o}(q/mc^2)(\omega_\alpha/c)e\sin\phi_s - \frac{3}{2}\frac{q/mc^2}{\beta_o^2\gamma_o}e'\cos\phi_s + \frac{3}{2}(1-\frac{\gamma_o^2}{2})\Big(\frac{(q/mc^2)e\cos\phi_s}{\beta_o^2\gamma_o^2}\Big)^2 \tag{2.94}$$

Now we can compute the equations for the linear map using $M' = JSM$. We will find that M breaks up into a separate 2×2 matrix for the horizontal, vertical, and temporal dimensions, and further, that each 2×2 block is a product of three matrices. The results are

$$\begin{pmatrix} \bar{x} \\ \bar{p}_x \end{pmatrix}^f = \begin{pmatrix} u^{-1/2} & 0 \\ -u^{1/2}\Delta & u^{1/2} \end{pmatrix}^f \begin{pmatrix} a_x & b_x \\ c_x & d_x \end{pmatrix}^f \begin{pmatrix} u^{1/2} & 0 \\ u^{1/2}\Delta & u^{-1/2} \end{pmatrix}^i \begin{pmatrix} \bar{x} \\ \bar{p}_x \end{pmatrix}^i \tag{2.95}$$

$$\begin{pmatrix} \bar{y} \\ \bar{p}_y \end{pmatrix}^f = \begin{pmatrix} u^{-1/2} & 0 \\ -u^{1/2}\Delta & u^{1/2} \end{pmatrix}^f \begin{pmatrix} a_y & b_y \\ c_y & d_y \end{pmatrix}^f \begin{pmatrix} u^{1/2} & 0 \\ u^{1/2}\Delta & u^{-1/2} \end{pmatrix}^i \begin{pmatrix} \bar{y} \\ \bar{p}_y \end{pmatrix}^i \tag{2.96}$$

$$\begin{pmatrix} \bar{\phi} \\ \bar{p}_\phi \end{pmatrix}^f = \begin{pmatrix} u^{-3/2} & 0 \\ -\frac{3l}{2}(\frac{u'}{u})u^{3/2} & u^{3/2} \end{pmatrix}^f \begin{pmatrix} a_\phi & b_\phi \\ c_\phi & d_\phi \end{pmatrix}^f \begin{pmatrix} u^{3/2} & 0 \\ \frac{3l}{2}(\frac{u'}{u})u^{3/2} & u^{-3/2} \end{pmatrix}^i \begin{pmatrix} \bar{\phi} \\ \bar{p}_\phi \end{pmatrix}^i \tag{2.97}$$

where the superscripts i and f denote initial and final values, respectively. Lastly, the quantities a_j,b_j,c_j, and d_j $(j = x, y, \phi)$ satisfy the following equations:

$$a'_j = c_j/l, \qquad b'_j = d_j/l, \tag{2.98}$$

$$c'_j = -l\Omega_j a_j, \qquad d'_j = -l\Omega_j b_j, \tag{2.99}$$

or equivalently,

$$a''_j + \Omega_j a_j = 0, \tag{2.100}$$

$$b''_j + \Omega_j b_j = 0, \tag{2.101}$$

with initial values $a_j = d_j = 1$, $b_j = c_j = 0$.

2.5 Courant-Snyder Theory

Designing and optimizing beam transport systems depends heavily on one's ability to compute and analyze maps. In fact, in has been stated (by John Irwin of SLAC) that virtually all single-particle magnetic optics calculations, with the exception of predicting dynamic aperture,

can be done *analytically*. Lie algebraic methods in accelerator physics (which were founded by Alex Dragt of the University of Maryland and further developed by Dragt, Etienne Forest, and others) provide a complete framework for the linear and nonlinear computation and analysis of maps. But long before the advent of Lie methods, the *linear* theory of Courant and Snyder was well known. Courant-Snyder theory provides a means to begin studying periodic transport systems without first having to learn Lie methods. Furthermore it does this in an environment familiar to most people, since it involves only a basic knowledge of linear ordinary differential equations.

Consider the following second order linear differential equation,

$$\frac{d^2x}{ds^2} + k(s)x = 0. \tag{2.102}$$

In the accelerator context, $k(s)$ would denote the linear focusing strength in a transport system, and for circular systems (which we will treat shortly) it would be periodic. But for now the following applies in general and not just to periodic systems.

The solution of the above equation can be expressed in terms of two functions $a(s)$ and $b(s)$, which satisfy Eq. (2.102), and initial values x_0 and x_0':

$$x(s) = x_0 a(s) + x_0' b(s) \tag{2.103}$$

$$x'(s) = x_0 a'(s) + x_0' b'(s), \tag{2.104}$$

or, in matrix notation,

$$\begin{pmatrix} x \\ x' \end{pmatrix}_s = \begin{bmatrix} a(s) & b(s) \\ a'(s) & b'(s) \end{bmatrix} \begin{pmatrix} x \\ x' \end{pmatrix}_0 \tag{2.105}$$

The 2×2 matrix M in the above equation is the linear transfer map that characterizes the system between locations 0 and s. Depending on the choice of these locations, M can denote the map for a single beamline element, a collection of elements, or an entire beam transport system. Note that M has unit determinant:

$$\det M = 1. \tag{2.106}$$

This is easy to demonstrate, since the initial value of M is unity, and it is easy to show that $d/ds\ (\det M) = 0$.

- **Problem 2.5** Prove that $d/ds\ (\det M) = 0$.

2.5.1 Invariant of Motion

Consider the time-independent Hamiltonian system,

$$H = \frac{p^2}{2} + k_o \frac{x^2}{2}, \tag{2.107}$$

where k_o is a constant. Obviously this system has an invariant (which is just the energy):

$$\frac{p^2}{2} + k_o \frac{x^2}{2} = constant. \tag{2.108}$$

When a particle evolves in this system, its moves continuously in phase space on an the ellipse specified by the preceding equation.

Now consider the *time-dependent* Hamiltonian,

$$H = \frac{p^2}{2} + k(s) \frac{x^2}{2}, \tag{2.109}$$

This system also has an exact invariant,

$$I = \frac{x^2}{w^2} + (wx' - xw')^2, \tag{2.110}$$

where a prime denotes d/ds, and where w satisfies the equation

$$w'' + k(s)w - \frac{1}{w^3} = 0. \tag{2.111}$$

- **Problem 2.6** Prove that $dI/ds = 0$.

Now define quantities β and α according to

$$\beta = w^2, \tag{2.112}$$

$$\alpha = -ww'. \tag{2.113}$$

Then I can be rewritten as

$$I = \frac{1}{\beta}\left[x^2 + (\alpha x + \beta x')^2\right]. \tag{2.114}$$

Lastly, if we define a quantity γ according to

$$\beta\gamma - \alpha^2 = 1, \tag{2.115}$$

we obtain

$$I = \gamma x^2 + 2\alpha x x' + \beta (x')^2. \tag{2.116}$$

The quantity I is the Courant-Snyder invariant.

2.5.2 Solution of the Equations of Motion

Given the time-dependent system with equation of motion

$$x'' + k(s)x = 0, \tag{2.117}$$

let

$$x(s) = w(s)e^{\pm i\psi(s)}. \tag{2.118}$$

It is easy to show that this is a solution provided that w and ψ satisfy

$$w'' + k(s)w - \frac{1}{w^3} = 0, \tag{2.119}$$

$$\psi' = \frac{1}{w^2}. \tag{2.120}$$

- **Problem 2.7** Prove the previous assertion.

It follows that the general solution for x is given by

$$x = Aw\cos\psi + Bw\sin\psi, \tag{2.121}$$

where A and B are constants. Two important points are the following:

1. This motion is not harmonic (except if $k(s) = constant$), but only pseudoharmonic, since w and ψ are generally functions of s.

2. The statement is often made that an s-dependent transport system can be "transformed into" one with constant focusing. This can be understood in terms of the preceding analysis. From Eq. (2.118) it is evident that, if we treat the quantity x/w as a dynamical variable that evolves as a function of ψ, then its motion is harmonic, with period 2π, and it must satisfy the equation

$$\frac{d^2(x/w)}{d\psi^2} + (x/w) = 0. \tag{2.122}$$

- **Problem 2.8** Show that

$$\frac{d(x/w)}{d\psi} = wx' - xw', \tag{2.123}$$

where a prime denotes d/ds. Use this to derive Eq. (2.122).

Assume without loss of generality that $\psi(0) = 0$. It follows from the initial values that

$$A = x_0/w_0, \tag{2.124}$$

$$B = w_0 x_0' - x_0 w_0'. \tag{2.125}$$

The complete solution for $x(t)$, $x'(t)$ is given by

$$\begin{pmatrix} x \\ x' \end{pmatrix}_s = M \begin{pmatrix} x \\ x' \end{pmatrix}_0, \tag{2.126}$$

where M is given by

$$\begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} = \begin{bmatrix} \frac{w(s)}{w_0}\cos\psi(s) - w(s)w_0'\sin\psi(s) & w_0 w(s)\sin\psi(s) \\ dm_{11}/ds & dm_{12}/ds \end{bmatrix} \tag{2.127}$$

This holds for arbitrary s. Now consider a periodic transport system and evaluate this for one period of the system, $s = L$. That is, let $w(L) = w(0) = w$, and let $\psi(L) = \mu$. It follows that

$$M = \begin{bmatrix} \cos\mu - ww'\sin\mu & w^2\sin\mu \\ -\frac{1+(ww')^2}{w^2}\sin\mu & \cos\mu + ww'\sin\mu \end{bmatrix} \tag{2.128}$$

Making use of the previous definitions for α, β, and γ, we finally obtain

$$M = \begin{bmatrix} \cos\mu + \alpha\sin\mu & \beta\sin\mu \\ -\gamma\sin\mu & \cos\mu - \alpha\sin\mu \end{bmatrix} \tag{2.129}$$

This is the one-period map for a stable, periodic, symplectic system in one dimension. The quantities α, β, and γ are *linear lattice functions*, and μ is the phase shift per period.

The β-function, $\beta = w^2$, is particularly important in periodic systems. This can be seen from Eq. (2.122), which can be rewritten as

$$x = \frac{w}{\sqrt{(A^2 + B^2}}\cos(\psi - \theta), \tag{2.130}$$

where $\tan\theta = B/A$. Since w is a periodic function of s, when a particle makes a complete revolution only the phase term in the preceding equation can change, and this term varies between ± 1. Thus, w is proportional to the maximum excursion that a particle can have at a given location s. Since a beam of particles will have all phases, it follows that w is equal to the beam envelope (up to a multiplicative constant).

- **Problem 2.9** Prove that the eigenvalues of the one-period map are $\exp(\pm i\mu)$. Find the corresponding eigenvectors.

Chapter 3

Lie Algebraic Methods

Lie Algebraic methods provide a powerful framework in which to analyze the motion of charged particles in accelerators and beam transport systems. The father of Lie methods in accelerator physics, Alex Dragt, began developing these tools in the late 1970's [10]. They were originally greeted with skepticism by some in the accelerator community who felt that the mathematics was too complicated. But over time the situation has changed, and Lie methods are now recognized as a natural, powerful framework for the design and analysis of nonlinear dynamics in Hamiltonian systems.

It is not the purpose of these notes to provide a comprehensive exposition on Lie algebraic methods. For that, the reader should see the many references, for example [10],[11], [12],[13], [14],[16]. Instead, these notes are meant to provide an overview of the basic tools and enough information to begin using Lie methods to solve basic beam dynamics problems.

3.1 Symplectic Matrices and Symplectic Mappings

Let M denote a $2m \times 2m$ matrix. Let J denote the $2m \times 2m$ matrix given by.

$$J = \begin{pmatrix} J_1 & 0 & 0 & 0 \\ 0 & J_1 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & J_1 \end{pmatrix}, \tag{3.1}$$

where J_1 is the 2×2 matrix given by

$$J_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{3.2}$$

The matrix M is said to be a *symplectic matrix* if it satisfies

$$\tilde{M} J M = J. \tag{3.3}$$

Symplectic matrices have several important properties that we state here (see, for example, [10]):

1. $\det M = 1$.
2. The eigenvalues of M are real or they occur in complex conjugate pairs.
3. If λ is an eigenvalue of M, then so is $1/\lambda$.
4. The real dimensionality of M (i.e. the number of real parameters necessary to specify an arbitrary $2m \times 2m$ symplectic matrix) is $m(2m+1)$.
5. The set of $2m \times 2m$ symplectic matrices forms a group, Sp(2m).

Another important property is related to the *normal form* of a symplectic matrix. A common concept from linear algebra is that, given a real symmetric matrix, it is possible to perform a similarity transformation that transforms it to a diagonal matrix with eigenvalues on the

diagonal. Analogously, it is possible to perform a similarity transformation on a symplectic matrix that transforms it into a special form. To connect this to beam dynamics, consider an m-dimensional ($2m$ degree-of-freedom) periodic system, and suppose that the linear dynamics of the system is described by a symplectic matrix M. Suppose that the motion is stable in all m dimensions. Then it is possible to perform a symplectic similarity transformation which turns M into a matrix consisting of 2×2 rotation matrices along the diagonal, and zeros elsewhere. In other words, there exists a symplectic matrix A such that

$$A^{-1}MA = N, \tag{3.4}$$

where

$$N = \begin{pmatrix} R(\mu_1) & 0 & 0 & 0 \\ 0 & R(\mu_2) & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & R(\mu_n) \end{pmatrix}, \tag{3.5}$$

and where

$$R(\mu_i) = \begin{pmatrix} \cos\mu_i & \sin\mu_i \\ -\sin\mu_i & \cos\mu_i \end{pmatrix}. \tag{3.6}$$

Here the eigenvalues of M are $e^{\pm i\mu_i}$. For a periodic system, the eigenvalues are related to quantities of physical interest. Namely, μ_i equals the phase shift per period or the phase shift per cell in the ith dimension.

So far we have discussed symplectic matrices. Now we will discuss symplectic mappings. Let ζ denote a vector with $2m$ components, and let $\mathcal{M}$ denote a mapping that maps an initial set of variables, ζ^{in} into a final set of variables ζ^{fin}:

$$\mathcal{M} : \zeta^{in} \rightarrow \zeta^{fin}. \tag{3.7}$$

Let M denote the Jacobian matrix of $\mathcal{M}$:

$$M_{ab} = \frac{\partial \zeta_a^{fin}}{\partial \zeta_b^{in}} \qquad (a, b = 1, \ldots, 2m). \tag{3.8}$$

Then $\mathcal{M}$ is said to be a *symplectic mapping* if its Jacobian is a symplectic matrix.

Now that we have laid the groundwork, we can discuss the relationship between symplectic mappings and Hamiltonian systems.

3.2 Symplectic Mappings and Hamiltonian Dynamics

Consider a Hamiltonian system with Hamiltonian $H(\vec{q},\vec{p})$. Recall that

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \tag{3.9}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \tag{3.10}$$

Now let $\zeta = (q_1, p_1, q_2, p_2, \ldots, q_m, p_m)$. Hamilton's equations can be rewritten in the form

$$\dot{\zeta} = J\partial_{\vec{\zeta}} H, \tag{3.11}$$

where

$$\partial_{\vec{\zeta}} H = \begin{pmatrix} \frac{\partial H}{\partial \zeta_1} \\ \vdots \\ \frac{\partial H}{\partial \zeta_{2m}} \end{pmatrix}. \tag{3.12}$$

The relevance of symplectic dynamics to analyzing the motion of charged particles in accelerators is due to the following fact:

All Hamiltonian flows are symplectic mappings

We now provide a sketch of the proof of this statement, following Dragt [10]. First divide the time interval from t^{in} to t^{fin} into N steps of length h, and regard the map $\mathcal{M}$ as being made up of a succession of N mappings:

$$\mathcal{M} = \mathcal{M}^{t_N \leftarrow t_{N-1}} \mathcal{M}^{t_{N-1} \leftarrow t_{N-2}} \cdots \mathcal{M}^{t_2 \leftarrow t_1} \mathcal{M}^{t_1 \leftarrow t_0} \tag{3.13}$$

where $t^0 = t^{in}$ and $t^N = t^{fin}$. By the chain rule, the associated Jacobian matrix is given by

$$M = M^{t_N \leftarrow t_{N-1}} M^{t_{N-1} \leftarrow t_{N-2}} \cdots M^{t_2 \leftarrow t_1} M^{t_1 \leftarrow t_0} \tag{3.14}$$

Next we will show that $M^{t^{n+1} \leftarrow t^n}$ is symplectic through order h. First, by Taylor's theorem,

$$\zeta^{n+1} = \zeta^n + h\dot{\zeta}^n + O(h^2). \tag{3.15}$$

Substituting Eq. (3.11), we obtain

$$\zeta^{n+1} = \zeta^n + hJ\partial_{\tilde{\zeta}} H + O(h^2), \tag{3.16}$$

or, in component form,

$$\zeta_a^{n+1} = \zeta_a^n + h\sum_{c=1}^{2n} J_{ac}\frac{\partial H}{\partial \zeta_c} + O(h^2), \tag{3.17}$$

The Jacobian of this transformation is found by taking $\partial/\partial\zeta_b$:

$$M_{ab}^{t^{n+1}\leftarrow t^n} = \delta_{ab} + h\sum_{c=1}^{2n} J_{ac}\frac{\partial^2 H}{\partial\zeta_b\,\partial\zeta_c} + O(h^2), \tag{3.18}$$

or

$$M^{t^{n+1}\leftarrow t^n} = I + hJS + O(h^2), \tag{3.19}$$

where I is the identity matrix, and where S is a symmetric matrix given by

$$S_{ab}\frac{\partial^2 H}{\partial\zeta_a\,\partial\zeta_b}. \tag{3.20}$$

Next, we check the symplectic condition, $\tilde{M}JM = J$:

$$\tilde{M}^{t^{n+1}\leftarrow t^n} J M^{t^{n+1}\leftarrow t^n} = \left[I - hSJ + O(h^2)\right] J \left[I + hJS + O(h^2)\right] = J + O(h^2), \tag{3.21}$$

where we have made use of the relations

$$\begin{aligned} J^2 &= -I, \\ \tilde{J} &= -J. \end{aligned} \tag{3.22}$$

Applying this same argument to Eq. (3.14) we find that

$$\tilde{M}JM = J + O(Nh^2) = J + O(Th), \tag{3.23}$$

since $Nh^2 = hT$, where $T = t^{fin} - t^{in} = Nh$. It follows that

$$\lim_{h\to 0, N\to\infty} \tilde{M}JM = J. \tag{3.24}$$

Hence $\mathcal{M}$ is a symplectic mapping.

Symplectic maps have many important properties, two of which we will discuss here: Liouville's theorem, and the preservation of Poisson brackets.

Consider an ensemble of noninteracting particles, each governed by the same Hamiltonian $H(\zeta, t)$. At some time t^{in} suppose that all of the particles occupy a region R^{in} of phase space with volume v^{in}:

$$V^{in} = \int_{R^{in}} d\vec{\zeta}^{in} \tag{3.25}$$

Now let the particles evolve to some later time t^{fin}, and let R^{fin} denote the region of phase space occupied by the particles at t^{fin}. The volume of this region is given by

$$V^{fin} = \int_{R^{fin}} d\vec{\zeta}^{fin} \tag{3.26}$$

Since ζ^{in} and ζ^{fin} are related by a symplectic mapping, the Jacobian determinant of the mapping equals one, and we obtain

$$V^{fin} = \int_{R^{fin}} d\vec{\zeta}^{fin} = \int_{R^{in}} |\frac{\partial \vec{\zeta}^{fin}}{\partial \vec{\zeta}^{in}}| d\vec{\zeta}^{in} = \int_{R^{in}} |\det M| d\vec{\zeta}^{in} = \int_{R^{in}} d\vec{\zeta}^{in} \tag{3.27}$$

Thus, $V^{fin} = V^{in}$, i.e. the volume of phase space occupied by an ensemble of particles is preserved as the system evolves in time. This is Liouville's theorem.

An alternative statement of Liouville's theorem is as follows: Since the number of particles occupying the region $R(t)$ is constant, and since the volume of the region is also constant, it follows that the phase space density (or distribution function) is preserved. That is, if $f(\zeta, t)$ is a distribution function on phase space, then it is constant along a trajectory,

$$f(\zeta^{in}, t^{in}) = f(\zeta^{fin}, t^{fin}) \tag{3.28}$$

Alternatively, we can write

$$\frac{df}{dt} = 0, \tag{3.29}$$

where d/dt denotes the *total* derivative along the flow (sometimes written at D/Dt).

A second important property of symplectic mappings is the preservation of Poisson brackets under time-evolution. Given any two functions $f(\zeta)$ and $g(\zeta)$, the Poisson bracket of f and g is given by

$$[f,g] = \sum_{i=1}^{m}(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}). \tag{3.30}$$

This can be rewritten

$$[f,g] = \sum_{a,b=1}^{2m}\frac{\partial f}{\partial \zeta_a}J_{ab}\frac{\partial g}{\partial \zeta_b}, \tag{3.31}$$

where J_{ab} was defined previously. More precisely, we can write

$$\Big[f(\zeta^f), g(\zeta^f)\Big]_{\zeta^f} = \sum_{a,b=1}^{2m}\frac{\partial f(\zeta^f)}{\partial \zeta_a^f}J_{ab}\frac{\partial g(\zeta^f)}{\partial \zeta_b^f}, \tag{3.32}$$

Now suppose we evaluate the Poisson bracket not in terms of the final variables but rather in terms of the initial variables:

$$\Big[f(\zeta^f), g(\zeta^f)\Big]_{\zeta^i} = \sum_{a,b=1}^{2m}\frac{\partial f(\zeta^f)}{\partial \zeta_a^i}J_{ab}\frac{\partial g(\zeta^f)}{\partial \zeta_b^i}, \tag{3.33}$$

If ζ^i and ζ^f are related by a symplectic mapping, then we can show that Eqs. (3.32) and (3.33) are equivalent: By the chain rule, Eq. (3.33) is equal to

$$\Big[f(\zeta^f), g(\zeta^f)\Big]_{\zeta^i} = \sum_{a,b=1}^{2m}\sum_{r,s=1}^{2m}\frac{\partial f(\zeta^f)}{\partial \zeta_r^f}\frac{\partial(\zeta_r^f)}{\partial \zeta_a^i}J_{ab}\frac{\partial g(\zeta^f)}{\partial \zeta_s^f}\frac{\partial(\zeta_s^f)}{\partial \zeta_b^i}. \tag{3.34}$$

The right-hand-side of this equation is simply

$$\sum_{a,b=1}^{2m}\sum_{r,s=1}^{2m}\frac{\partial f(\zeta^f)}{\partial \zeta_r^f}M_{ra}J_{ab}\tilde{M}_{bs}\frac{\partial g(\zeta^f)}{\partial \zeta_s^f} = \sum_{r,s=1}^{2m}\frac{\partial f(\zeta^f)}{\partial \zeta_r^f}J_{rs}\frac{\partial g(\zeta^f)}{\partial \zeta_s^f} \tag{3.35}$$

But this is just Eq. (3.32). Thus, the Poisson bracket of any two functions is preserved under symplectic mappings, and it does not matter whether we compute the bracket using the initial variables ζ^i or the final variables, ζ^f. Conversely, it can be shown that if a map $\mathcal{M}$ preserves the fundamental Poisson brackets, $[\zeta_a, \zeta_b] = J_{ab}$, then $\mathcal{M}$ is symplectic. We will use this property in the next sectioni, when we discuss the relationship of Lie transformations with symplectic mappings.

3.3 Lie Algebraic Tools

We have shown that the mappings generated by Hamiltonian flows are symplectic. This greatly restricts the mappings that we will deal with when analyzing the dynamics of particles in accelerators. (For now we neglect non-Hamiltonian processes such as synchrotron radiation.) It is wise to look for a representation of $\mathcal{M}$ that exploits this fundamental property about the nature of the map. This will lead us to a Lie algebraic representation of $\mathcal{M}$. First, we need to introduce some Lie algebraic tools.

Let $f(\zeta, t)$ be any function of the phase space variables, and perhaps the time. The Lie operator associated with f, denoted $: f :$, is defined by

$$: f : g = [f, g] \,, \tag{3.36}$$

for all $g(\zeta, t)$, where $[,]$ denotes the Poisson bracket. Several important properties of Lie operators, stated without proof, are the following:

1. Linearity:

$$a : f : + b : g :=: (af + bg) : \qquad a, b \; in \; \mathbf{R} \tag{3.37}$$

2. Derivation with respect to ordinary multiplication:

$$: f : (gh) = (: f : g)h + g(: f : h) \tag{3.38}$$

3. Derivation with respect to Poisson bracket multiplication:

$$: f : [g, h] = [: f : g, h] + [g, : f : h] \tag{3.39}$$

4. Lie operator associated with a commutator: Let $\{,\}$ denote the commutator of two Lie operators,

$$\{: f :, : g :\} \equiv : f :: g : - : g :: f : \tag{3.40}$$

   Then the above commutator is also a Lie operator, and its associated function is the Poisson bracket of f and g,

$$\{: f :, : g :\} =: [f, g] : \tag{3.41}$$

Now that we have defined Lie operators and listed some of their properties, we will define powers of Lie operators. This is easily done in terms of repeated applications of the Poisson bracket:

$$\begin{aligned} :f:^0 g &= g, \\ :f:^1 g &= [f,g], \\ :f:^2 g &= [f,[f,g]], \\ :f:^3 g &= [f,[f,[f,g]]], \\ &\vdots \end{aligned} \tag{3.42}$$

Having defined powers of Lie operators, we can now discuss power series of Lie operators. In particular, we can define *Lie transformations*, which are the key element in the Lie algebraic representation of transfer maps. The Lie transformation associated with f is simply $\exp(:f:)$,

$$e^{:f:} = \sum_{n=0}^{\infty} \frac{:f:^n}{n!}. \tag{3.43}$$

For example, the action of $\exp(:f:)$ on a function g is given by

$$e^{:f:}g = \sum_{n=0}^{\infty} \frac{:f:^n g}{n!} = g + :f:g + \frac{1}{2}:f:^2 g + \frac{1}{3!}:f:^3 g + \cdots \tag{3.44}$$

Using the properties of Lie operators listed earlier, one can show that Lie transformations have the following properties:

1. Linearity:
$$e^{:f:}(ag+bh) = ae^{:f:}g + be^{:f:}h \tag{3.45}$$

2. Isomorphism with respect to ordinary multiplication:
$$e^{:f:}(gh) = (e^{:f:}g)(e^{:f:}h) \tag{3.46}$$

3. Isomorphism with respect to Poisson bracket multiplication:
$$e^{:f:}[g,h] = \left[e^{:f:}g, e^{:f:}h\right] \tag{3.47}$$

4. Transformation of a function via its arguments:

$$e^{:f:}g(\zeta_1,\zeta_2,\ldots,\zeta_{2m}) = g(e^{:f:}\zeta_1, e^{:f:}\zeta_2,\ldots,e^{:f:}\zeta_{2m}) \tag{3.48}$$

5. "Sandwich Theorem":

$$e^{:f:}e^{:g:}e^{-:f:} = e^{e^{:f:}g} \tag{3.49}$$

The last two properties are extremely useful for manipulating maps.

At this point one might ask what all of this mathematical formalism has to do with beam dynamics? The answer lies in the following fact:

Every Lie transformation is a symplectic mapping

Thus, Lie methods provide a natural framework for representing and parameterizing symplectic maps. To see that Lie transformations are symplectic mappings, consider a map

$$\mathcal{M}(\zeta) = e^{:f(\zeta):} \tag{3.50}$$

that transforms ζ into ζ^{fin}:

$$\zeta^{fin} = \mathcal{M}(\zeta)\ \zeta. \tag{3.51}$$

It follows from the previously listed properties of Lie transformations that

$$\left[\zeta_a^{fin},\zeta_b^{fin}\right] = \left[e^{:f:}\zeta_a, e^{:f:}\zeta_b\right] = e^{:f:}\left[\zeta_a,\zeta_b\right] = e^{:f:}J_{ab} = J_{ab}. \tag{3.52}$$

Since $\mathcal{M}$ preserves the fundamental Poisson brackets, it is a symplectic mapping.

3.4 Successive Lie Transformations

Normally one is interested, not in a single mapping, but in the collection of mappings that make up part or all of a beamline. At first glance one might suppose, in a quantity like

$$e^{:f(\zeta):}e^{:g(\zeta):}, \tag{3.53}$$

that the map $e^{:g:}$ acts first, transforming ζ into an intermediate result, which is then acted upon by $e^{:f:}$. This interpretation is wrong. In the above expression, $e^{:f:}$ acts first, and $e^{:g:}$ acts second. That is, $e^{:f:}$ represents the first element encountered in the beamline, and $e^{:g:}$ represents the second. It is important to understand this, since the manipulation of Lie transformations is a powerful tool for the design and optimization of beamlines.

Consider two successive transformations,

$$\zeta_0 \xrightarrow{\mathcal{M}_1} \zeta_1 \xrightarrow{\mathcal{M}_2} \zeta_2, \tag{3.54}$$

where

$$\begin{aligned} \mathcal{M}_1 &= e^{:f_1:}, \\ \mathcal{M}_2 &= e^{:f_2:}. \end{aligned} \tag{3.55}$$

More explicitly,

$$\begin{aligned} \zeta_1 &= \mathcal{M}_1(\zeta_0)\zeta_0 = e^{:f_1(\zeta_0):}\zeta_0, \\ \zeta_2 &= \mathcal{M}_2(\zeta_1)\zeta_1 = e^{:f_1(\zeta_l):}\zeta_1. \end{aligned} \tag{3.56}$$

It follows that

$$\zeta_2 = \mathcal{M}_2(\zeta_1)\mathcal{M}_1(\zeta_0)\zeta_0. \tag{3.57}$$

This result "looks" correct, because if $\mathcal{M}_1$ and $\mathcal{M}_2$ were matrices, M_1 and M_2, we would write $\vec{\zeta_2} = M_2 M_1 \vec{\zeta_0}$. However, the above is misleading because not all of the variables on the right hand side are expressed in terms of ζ_0. If we do that, we obtain

$$\begin{aligned} \mathcal{M}_2(\zeta_1)\mathcal{M}_1(\zeta_0) = e^{:f_2(\zeta_1):}e^{:f_1(\zeta_0):} = \\ e^{:f_1(\zeta_0):}e^{-:f_1(\zeta_0):}e^{:f_2(\zeta_1):}e^{:f_1(\zeta_0):} = e^{:f_1(\zeta_0):}e^{:f_2(e^{-:f_1(\zeta_0):}\zeta_1):} \end{aligned} , \tag{3.58}$$

where we have made use of Eq. (3.49). Finally, making use of

$$e^{-:f_1(\zeta_0):}(\zeta_1) = \zeta_0, \tag{3.59}$$

which follows from inverting the first equation in (3.56), we obtain

$$\zeta_2 = e^{:f_1(\zeta_0):}e^{:f_2(\zeta_0):}\zeta_0 = \mathcal{M}_1(\zeta_0)\mathcal{M}_2(\zeta_0). \tag{3.60}$$

That is, the Lie transformations occur in *anti-chronological* order; one should regard the left-most map as acting first and the right-most map as acting last.

3.5 Representation of Transfer Maps

Consider an m-dimensional dynamical system governed by some Hamiltonian $H(\zeta, t)$, where $\zeta = (q_1, p_2, q_2, p_2, \ldots, q_m, p_m)$. An obvious method of representing $\mathcal{M}$ (or the action of $\mathcal{M}$ on ζ^{in}) is to expand ζ^{fin} as a power series in ζ^{in}:

$$\zeta_a^{fin} = \sum_{b=1}^{2m} M_{ab}\zeta_b^{in} + \sum_{1\le b\le c}^{2m} T_{abc}\zeta_b^{in}\zeta_c^{in} + \sum_{1\le b\le c\le d}^{2m} u_{abcd}\zeta_b^{in}\zeta_c^{in}\zeta_d^{in} + \cdots \quad (3.61)$$

(Here we have assumed that $\mathcal{M}$ maps the origin of phase space into itself, so there is no constant term in the expansion.) The linear behavior of $\mathcal{M}$ is represented by the matrix M, and the nonlinear behavior is governed by the tensors T, U, etc. For example, the tensor T governs second order nonlinear behavior, the tensor U governs third order behavior, and so on.

The above expansion is legitimate, but it has two drawbacks. First, the coefficients of M, T, U, etc., are not independent (whereas the expansion seems to imply that they may be chosen independently). In fact, they are linked by the symplectic condition. Thus, if we separately compute all the coefficients of M, T, U, etc., we are really doing more work than necessary. Second, if the Taylor series is truncated at some order, then the truncated series is generally not symplectic.

A useful Lie algebraic representation of $\mathcal{M}$ is given by

$$\mathcal{M} = e^{:f_2:}e^{:f_3:}e^{:f_4:}\cdots \quad (3.62)$$

That is, $\mathcal{M}$ is represented as an infinite product of Lie transformations. The quantities f_n are homogeneous polynomials of degree n in $q_1, p_1, q_2, p_2, \ldots, q_m, p_m$. For example, in one dimension the polynomial f_3 is of the form $ax^3+bx^2p_x+cxp_x^2+dp_x^3$. The proof of the *Factorization Theorem* is due to Dragt and Finn [15]. This representation of $\mathcal{M}$ has certain important features:

1. The quantity $e^{:f_2:}$ is a linear mapping. That is, there exists a matrix M (the same as in Eq. (3.61)), such that

$$e^{:f_2:}\vec{\zeta} = M\vec{\zeta}. \quad (3.63)$$

2. The polynomials $f_3, f_4, \ldots$ describe nonlinear effects. For example, f_3 is related to second order effects, f_4 is related to third order effects, and so on.

3. The polynomials $f_3, f_4, \ldots$ utilize the *minimum* number of coefficients to specify M up to a given order.

4. If the infinite product is truncated at some order, the remaining truncated product is still a symplectic mapping.

A representation of the map which correctly describes the dynamics though third order is obtained by dropping all terms beyond f_4,

$$\mathcal{M} = e^{:f_2:} e^{:f_3:} e^{:f_4:} \tag{3.64}$$

We can compare this with the Taylor representation by expanding the exponentials associated with f_3 and f_4, dropping terms beyond third order in ζ. (The term $e^{:f_2:}$ cannot be expanded, since each term in the expansion is of first order.) We obtain

$$\mathcal{M} = e^{:f_2:} \left[1 + : f_3 : + (\frac{1}{2} : f_3 :^2 + : f_4 :) \right] \tag{3.65}$$

In particular, the action of $\mathcal{M}$ on a component of ζ is given by

$$\mathcal{M}\zeta_a = e^{:f_2:}\zeta_a + e^{:f_2:} : f_3 : \zeta_a + e^{:f_2:}(\frac{1}{2} : f_3 :^2 + : f_4 :)\zeta_a \tag{3.66}$$

It is easy to associate these terms with the corresponding terms in the Taylor series:

$$e^{:f_2:}\zeta_a^{in} = \sum_{b=1}^{2m} M_{ab}\zeta_b^{in} \tag{3.67}$$

$$e^{:f_2:} : f_3 : \zeta_a^{in} = \sum_{1 \le b \le c}^{2m} T_{abc}\zeta_b^{in}\zeta_c^{in} \tag{3.68}$$

$$e^{:f_2:}(\frac{1}{2} : f_3 :^2 + : f_4 :)\zeta_a^{in} = \sum_{1 \le b \le c \le d}^{2m} u_{abcd}\zeta_b^{in}\zeta_c^{in}\zeta_d^{in} \tag{3.69}$$

It is worth emphasizing that the expanded Lie product and the Taylor series are *identical*; they contain the same physics, and, in expanded

form, neither is symplectic. The Lie polynomials contain the same information with fewer free parameters (in fact, the minimum number necessary). More importantly, knowing the Lie polynomials is often useful for fitting and optimizing maps to meet certain objectives.

Note that for some applications it is helpful to use the reverse factorization to that shown above. That is, there exist homogeneous polynomials g_n such that $\mathcal{M}$ has the representation

$$\mathcal{M} = \cdots e^{:g_4:} e^{:g_3:} e^{:g_2:} \tag{3.70}$$

Lastly, to represent a map through order $n-1$ in the Lie algebraic approach, one evidently needs a scheme to represent homogeneous polynomials through order n. The scheme that was adopted by Dragt and his coworkers is shown in an appendix. For polynomials in six variables (applicable to beam dynamics in three dimensions), the ordering is as follows: Entries 1-6 consist of first order monomials x, p_x, y, p_y, t, p_t; entries 7-27 contain the second order monomials $x^2, xp_x, \ldots, p_t^2$; entries 28-83 contain third order monomials $x^3, x^2p_x, \ldots, p_t^3$; entries 84-209 contain fourth order monomials $x^4, x^3p_x, \ldots, p_t^4$;

3.6 Computation of Lie Algebraic Maps

So far we have shown that (1) Hamiltonian flows generate symplectic maps, and (2) every symplectic map has a unique Lie algebraic representation

$$\mathcal{M} = \cdots e^{:g_4:} e^{:g_3:} e^{:g_2:} \tag{3.71}$$

Now we will discuss how to compute the polynomials g_2, g_3, g_4 for a given Hamiltonian system. This procedure was developed by Dragt and Forest [16]. Assume that we have already expanded the Hamiltonian around the reference trajectory, so that we can write

$$H = H_2 + H_3 + H_4 + \cdots \tag{3.72}$$

As already mentioned, the linear transfer map M, corresponding to g_2, satisfies the equation

$$\dot{M} = JSM, \tag{3.73}$$

where S is the symmetric matrix related to H_2,

$$H_2 = \frac{1}{2}\sum_{ab=1}^{2m} S_{ab}\zeta_a\zeta_b, \tag{3.74}$$

and where $J_{ab} = [\zeta_a, \zeta_b]$. Dragt and Forest also derived equations for the quantities g_3 through g_6. In particular,

$$\dot{g}_3 = -H_3^{int}, \tag{3.75}$$

$$\dot{g}_4 = -H_4^{int} - \frac{1}{2}\left[f_3, H_3^{int}\right], \tag{3.76}$$

where the interaction Hamiltonian is defined according to

$$H_n^{int} = H_n(M\zeta). \tag{3.77}$$

That is, H_n^{int} is obtain from H_n by transforming its arguments with the matrix M.

Using these formulas it is possible to compute transfer maps in the Lie algebraic representation. For simple Hamiltonians this can be done analytically, while for complicated Hamiltonians (e.g. z-dependent Hamiltonians such as those corresponding to beamline elements with realistic fringe fields), these equations must be solved numerically.

In closing we should mention the following: Lie methods provide an excellent means to analyze and manipulate maps. The above equations also provide an easy-to-implement scheme to compute maps. However, the formulas for $\dot{g}_n$ become increasingly complicated when extended to higher order. In contrast, the coefficients in the Taylor map can be obtained to arbitrarily high order using automatic differentiation and differential algebraic techniques [17]. For this reason, very high order maps are often calculated using the Taylor representation; if the Lie map is needed for analysis, it can be extracted from the Taylor map using standard tools.

Chapter 4

Multiparticle Dynamics

4.1 The Vlasov Equation

So far we have discussed the beam dynamics of individual particles. We found that the evolution of a particle with canonical coordinates and moment $\zeta = (x, p_x, y, p_y, z, p_z)$, from t^{in} to t^{fin}, is governed by a symplectic mapping, $\mathcal{M}$, where

$$\zeta^{fin} = \mathcal{M}\zeta^{in}. \tag{4.1}$$

The methods introduced previously also provide a means to analyze a distribution of interacting particles in the mean field approximation. Consider of beam of particles governed by a distribution function $f(\zeta, t)$. In the absence of particle-particle collisions, the distribution function satisfies the equation

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_j \frac{\partial f}{\partial \zeta_j}\frac{\partial \zeta_j}{\partial t} = 0, \tag{4.2}$$

or equivalently,

$$\frac{df}{dt} = -\left[H, f\right] = 0. \tag{4.3}$$

We will often be interested in cases for which H is of the form

$$H = H_{ext} + H_{self}, \tag{4.4}$$

where H_{ext} includes kinematic terms and terms related to externally applied fields, and H_{self} includes the self-fields. Frequently the self-fields are essentially electrostatic (in beam frame), and so the fields can be found by solving Poisson's equation,

$$\nabla^2\phi = -\rho/\epsilon_o. \tag{4.5}$$

In this case the above evolution equation for $f(\zeta, t)$, coupled with the Poisson equation, is known as the Vlasov/Poisson system.

The evolution of the distribution function can be expressed in terms of the transfer map, $\mathcal{M}$, and the initial distribution function, as shown: Let the initial distribution function be given by

$$f^o(\zeta) \equiv f(\zeta, t = t^{in}). \tag{4.6}$$

Then the time-evolved distribution function is given by

$$f(\zeta, t) = f^o(\mathcal{M}^{-1}\zeta). \tag{4.7}$$

That is, the time-evolved distribution function is equal to the initial distribution function with its arguments transformed by $\mathcal{M}^{-1}$. To see this, note that, because $df/dt = 0$, we can write

$$f(\zeta^{fin}, t^{fin}) = f(\zeta^{in}, t^{in}) = f^o(\zeta^{in}). \tag{4.8}$$

Substituting $\zeta^{in} = \mathcal{M}^{-1}\zeta^{fin}$, we obtain

$$f(\zeta^{fin}, t^{fin}) = f^o(\mathcal{M}^{-1}\zeta^{fin}), \tag{4.9}$$

which is equivalent to the advertised result.

One application of this is that it leads to a simple derivation of the KV equations, as described in the next section.

4.2 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

$$f(x, p_x, y, p_y) = \delta(Q(x, p_x, y, p_y)), \tag{4.10}$$

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,

$$f^o(x, p_x, y, p_y) = C\delta(\frac{x^2}{\sigma_x^2} + \frac{p_x^2}{\lambda_x^2} + \frac{y^2}{\sigma_y^2} + \frac{p_y^2}{\lambda_y^2}). \tag{4.11}$$

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

$$C = \frac{1}{\pi^2 \sigma_x \sigma_y \lambda_x \lambda_y}. \tag{4.12}$$

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

$$M = \begin{pmatrix} a_x & b_x & 0 & 0 \\ c_x & d_x & 0 & 0 \\ 0 & 0 & a_y & b_y \\ 0 & 0 & c_y & d_y \end{pmatrix}, \tag{4.13}$$

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

$$\rho(x,y) = \int\int d\vec{p} f^o(M^{-1}\zeta), \tag{4.14}$$

or,

$$\rho(x,y) = \int\int d\vec{p}\delta\left[\frac{(d_x x - b_x p_x)^2}{\sigma_x^2} + \cdots + \frac{(-c_y y + a_y p_y)^2}{\lambda_y^2}\right]. \tag{4.15}$$

The integrations can be performed using the substitutions

$$\begin{aligned} q\cos\theta &= p_x\sqrt{\frac{b_x^2}{\sigma_x^2}+\frac{a_x^2}{\lambda_x^2}} - x(\frac{b_x d_x}{\sigma_x^2}+\frac{a_x c_x}{\lambda_x^2})/\sqrt{\frac{b_x^2}{\sigma_x^2}+\frac{a_x^2}{\lambda_x^2}} \\ q\sin\theta &= p_y\sqrt{\frac{b_y^2}{\sigma_y^2}+\frac{a_y^2}{\lambda_y^2}} - y(\frac{b_y d_y}{\sigma_y^2}+\frac{a_y c_y}{\lambda_y^2})/\sqrt{\frac{b_y^2}{\sigma_y^2}+\frac{a_y^2}{\lambda_y^2}} \end{aligned} \tag{4.16}$$

Performing the integration, we obtain

$$\rho(x,y) = \frac{1}{\pi r_x r_y} \times \left\{ \begin{array}{ll} 1 & \text{if} \quad \frac{x^2}{r_x^2}+\frac{y^2}{r_y^2} < 1 \\ 0 & \text{if} \quad \frac{x^2}{r_x^2}+\frac{y^2}{r_y^2} > 1 \end{array} \right\}, \tag{4.17}$$

where

$$r_x^2 = \sigma_x^2 a_x^2 + \lambda_x^2 b_x^2, \qquad r_y^2 = \sigma_y^2 a_y^2 + \lambda_y^2 b_y^2. \tag{4.18}$$

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

$$\frac{x^2}{r_x^2} + \frac{y^2}{r_y^2} = 1. \tag{4.19}$$

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

$$\psi(x,y) = \frac{-\lambda}{2\pi\epsilon_o}\left[\frac{x^2}{r_x(r_x+r_y)} + \frac{y^2}{r_y(r_x+r_y)}\right] \qquad (\frac{x^2}{r_x^2} + \frac{y^2}{r_y^2} < 1) \quad (4.20)$$

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

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = -\frac{\lambda}{\pi\epsilon_o r_x r_y} \quad (4.21)$$

as required. Also, using

$$\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial^2 A_z}{\partial y^2} = -\mu_o\rho v_o, \quad (4.22)$$

we obtain

$$A_z = \frac{v_o}{c^2}\psi. \quad (4.23)$$

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

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{qg(z)}{2p^o}(x^2 - y^2) + \frac{q}{p^o v_o}\psi - \frac{q}{p^o}A_z. \quad (4.24)$$

It follows that

$$H = \frac{1}{2}(p_x^2+p_y^2) + \frac{k(z)}{2}(x^2-y^2) - K\left[\frac{x^2}{r_x(r_x+r_y)} + \frac{y^2}{r_y(r_x+r_y)}\right] \quad (4.25)$$

where

$$k(z) = \frac{q}{p^o}g(z), \quad (4.26)$$

and where

$$K = \frac{q\lambda}{2\pi\epsilon_o p^o v_o \gamma_o^2} \quad (4.27)$$

is the so-called generalized perveance.

Using Eq. (2.16), the matrix S associated with this Hamiltonian is

$$S = \begin{pmatrix} s_{11} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & s_{33} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{4.28}$$

where

$$\begin{aligned} s_{11} &= k - \frac{2K}{r_x(r_x + r_y)} \\ s_{33} &= -k - \frac{2K}{r_y(r_x + r_y)} \end{aligned} \tag{4.29}$$

$$\tag{4.30}$$

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

$$\begin{array}{cc} a_x' = c_x & a_y' = c_y \\ b_x' = d_x & b_y' = d_y \\ c_x' = -a_x\left[k - \frac{2K}{r_x(r_x+r_y)}\right] & c_y' = -a_y\left[-k - \frac{2K}{r_y(r_x+r_y)}\right] \\ d_x' = -b_x\left[k - \frac{2K}{r_x(r_x+r_y)}\right] & d_y' = -b_y\left[-k - \frac{2K}{r_y(r_x+r_y)}\right] \end{array} \tag{4.31}$$

These can be combined into four second order equations,

$$\begin{aligned} a_x'' + a_x\left[k - \frac{2K}{r_x(r_x + r_y)}\right] &= 0, \\ b_x'' + b_x\left[k - \frac{2K}{r_x(r_x + r_y)}\right] &= 0, \\ a_y'' + a_y\left[-k - \frac{2K}{r_y(r_x + r_y)}\right] &= 0, \\ b_y'' + b_y\left[-k - \frac{2K}{r_y(r_x + r_y)}\right] &= 0. \end{aligned} \tag{4.32}$$

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,

$$\begin{aligned} r_x'' + kr_x - \frac{2K}{(r_x + r_y)} - \epsilon_x^2/r_x^3 &= 0, \\ r_y'' - kr_y - \frac{2K}{(r_x + r_y)} - \epsilon_y^2/r_x^3 &= 0, \end{aligned} \tag{4.33}$$

where ϵ_x and ϵ_y denote the edge emittances

$$\begin{aligned} \epsilon_x &= \sigma_x \lambda_x, \\ \epsilon_y &= \sigma_y \lambda_y. \end{aligned} \tag{4.34}$$

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

$$f^o(x, p_x, y, p_y) = C\delta(\frac{x^2}{\sigma_x^2} + \frac{2\mu_x}{\sigma_x \lambda_x} x p_x + \frac{p_x^2}{\lambda_x^2} + \frac{y^2}{\sigma_y^2} + \frac{2\mu_y}{\sigma_y \lambda_y} y p_y + \frac{p_y^2}{\lambda_y^2}), \tag{4.35}$$

where

$$C = \frac{\sqrt{1-\mu_x^2}\sqrt{1-\mu_y^2}}{\pi^2 \sigma_x \sigma_y \lambda_x \lambda_y}. \tag{4.36}$$

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

$$\begin{aligned} \epsilon_x &= \frac{\sigma_x \lambda_x}{\sqrt{1-\mu_x^2}}, \\ \epsilon_y &= \frac{\sigma_y \lambda_y}{\sqrt{1-\mu_y^2}}. \end{aligned} \tag{4.37}$$

- **Problem 4.1**
  Derive the KV equations as described above.

- **Problem 4.2**
  Starting with Eq. (4.11), integrate the distribution function over y and p_y to obtain a function of x and p_x only. You will find that the function is constant inside an ellipse, and zero outside the ellipse. Show that the area of the ellipse is given by $A_x = \pi\sigma_x\lambda_x$. This demonstrates that, for a KV distribution, the horizontal edge emittance $\sigma_x\lambda_x$ is equal to the area of the ellipse in horizontal phase space divided by π. (An analogous statement obviously holds for the vertical phase space as well.)

4.3 RMS Equations

RMS envelope equations were first introduced by Sacherer and Lapostolle [20] [21]. An extensive treatment of cylindrically symmetric systems was given by Lee and Cooper [22]. 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.

4.3.1 Overview

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

$$A_x = A_y = 0, \tag{4.38}$$

$$A_z = \frac{1}{2} g(z)(y^2 - x^2), \tag{4.39}$$

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

$$A_x = A_y = 0, \tag{4.40}$$

$$A_z = \frac{\beta_o}{c}\Psi, \tag{4.41}$$

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

$$\bar{x} = x/l, \qquad \bar{p}_x = p_x/p_o, \tag{4.42}$$

$$\bar{y} = y/l, \qquad \bar{p}_y = p_y/p_o, \tag{4.43}$$

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

$$H(\bar{x}, \bar{p}_x, \bar{y}, \bar{p}_y; z) = \frac{1}{2l}(\bar{p}_x^2 + \bar{p}_y^2) + \frac{lk(z)}{2}(\bar{x}^2 - \bar{y}^2) + \frac{K/2}{l}\hat{\Psi}(l\bar{x}, l\bar{y}, z), \tag{4.44}$$

where

$$k(z) = (q/p_o)g(z), \tag{4.45}$$

and where K is the generalized perveance,

$$K = \frac{qI}{2\pi\epsilon_o p_o v_o^2 \gamma_o^2}. \tag{4.46}$$

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

$$\Psi = \frac{\lambda}{4\pi\epsilon_o}\hat{\Psi}, \tag{4.47}$$

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

$$H(x, p_x, y, p_y; z) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{k(z)}{2}(x^2 - y^2) + \frac{K}{2}\hat{\Psi}(lx, ly, z), \tag{4.48}$$

and the resulting equations of motion are

$$\begin{aligned} x' &= p_x, & (4.49)\\ p_x' &= -kx - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial x}, & (4.50)\\ y' &= p_y, & (4.51)\\ p_y' &= ky - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial y}, & (4.52) \end{aligned}$$

where a prime denotes d/dz.

4.3.2 Derivation of RMS Equations

Let X and Y denote the rms envelopes,

$$\begin{aligned} X &= \sqrt{< x^2 >}, \\ Y &= \sqrt{< y^2 >}, \end{aligned} \tag{4.53}$$

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

$$X' = \frac{< xx' >}{\sqrt{< x^2 >}} = \frac{< xp_x >}{X}. \tag{4.54}$$

Differentiating again, we obtain

$$X'' = -\frac{< xp_x > X'}{X^2} + \frac{< x'p_x + xp'_x >}{X}. \tag{4.55}$$

After some manipulation we obtain

$$X'' = \frac{< xp'_x >}{X} + \frac{\epsilon_x^2}{X^3}, \tag{4.56}$$

where the horizontal rms emittance is given by

$$\epsilon_x^2 =< x^2 >< p_x^2 > - < xp_x >^2 . \tag{4.57}$$

Substituting Eq. (4.50), we obtain

$$X'' + kX + \frac{(K/2)}{X} < x\frac{\partial\hat{\Psi}}{\partial x} > -\frac{\epsilon_x^2}{X^3} = 0. \tag{4.58}$$

All that remains is to compute $< x\frac{\partial\hat{\Psi}}{\partial x} >$. To do this, we will follow Sacherer [20] and assume that the beam density has elliptical symmetry:

$$\rho(x, y) = \rho\left(\frac{x^2}{a^2} + \frac{y^2}{b^2}\right). \tag{4.59}$$

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

$$\int_{-\infty}^{\infty} dx\ dy\ \rho\left(\frac{x^2}{a^2} + \frac{y^2}{b^2}\right) = 1, \tag{4.60}$$

it follows that

$$ab\int_0^{\infty} 2\pi r\ dr\ \rho(r^2) = 1. \tag{4.61}$$

By a similar calculation,

$$\begin{aligned} \sqrt{< x^2 >} &= aC, \\ \sqrt{< y^2 >} &= bC, \end{aligned} \tag{4.62}$$

where

$$C = \pi ab \int_0^\infty \; r^3 \; dr \; \rho(r^2). \tag{4.63}$$

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

Now consider Poisson's equation,

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} = -\lambda \rho / \epsilon_o, \tag{4.64}$$

where, as mentioned previously, λ is the charge per unit length. Given the distribution (4.59), we can write the solution of Poisson's equation formally as,

$$\Psi = -\frac{ab}{4\epsilon_o} \int_0^\infty ds \; \frac{\eta\left(\frac{x^2}{a^2+s} + \frac{y^2}{b^2+s}\right)}{\sqrt{a^2+s}\sqrt{b^2+s}}, \tag{4.65}$$

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

$$< x \frac{\partial \hat{\Psi}}{\partial x} >= -2\pi ab \int_{-\infty}^\infty dx \int_{-\infty}^\infty dy \int_0^\infty ds \; \frac{x^2 \rho\left(\frac{x^2}{a^2+s} + \frac{y^2}{b^2+s}\right)}{(a^2+s)^{3/2}(b^2+s)^{1/2}} \rho\left(\frac{x^2}{a^2} + \frac{y^2}{b^2}\right) \tag{4.66}$$

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

$$\begin{aligned} r\cos\theta &= \frac{x}{\sqrt{a^2+s}}, \\ r\sin\theta &= \frac{y}{\sqrt{b^2+s}}, \end{aligned} \tag{4.67}$$

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

$$r'^2 = r^2 \left[1 + s\left(\frac{\cos^2\theta}{a^2} + \frac{\sin^2\theta}{b^2}\right)\right]. \tag{4.68}$$

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

$$\int_0^{2\pi} d\theta \; \frac{\cos^2\theta}{\frac{\cos^2\theta}{a^2}+\frac{\sin^2\theta}{b^2}} = 2\pi ab\frac{a}{a+b}, \tag{4.69}$$

we obtain

$$< x\frac{\partial\hat{\Psi}}{\partial x} >= \frac{-2a^3b^2}{a+b}\int_0^\infty dr \; \rho(r^2)2\pi r \int_r^\infty dr' \; \rho(r'^2)2\pi r'. \tag{4.70}$$

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

$$F(r) = ab\int_0^r \rho(r^2)2\pi r \; dr, \tag{4.71}$$

where, from Eq. (4.61), $F(\infty) = 1$. Then we can write

$$< x\frac{\partial\hat{\Psi}}{\partial x} >= -2\frac{a}{a+b}\int_0^\infty dr \; \frac{dF}{dr}\left(1-F(r)\right). \tag{4.72}$$

This can be integrated to yield

$$< x\frac{\partial\hat{\Psi}}{\partial x} >= \frac{-a}{a+b} = \frac{-X}{X+Y}, \tag{4.73}$$

where we have used Eqs. (4.62) in the final equality. It follows that the rms envelope equations for a beam in a quadrupole channel are given by [20, 21]

$$\begin{aligned} &\frac{d^2X}{dz^2} + kX - \frac{K/2}{X+Y} - \frac{\mathcal{E}_x^2}{X^3} = 0, \\ &\frac{d^2Y}{dz^2} - kY - \frac{K/2}{X+Y} - \frac{\mathcal{E}_y^2}{Y^3} = 0, \end{aligned} \tag{4.74}$$

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

$$H^{\rm env}(X,P_x,Y,P_y) = \frac{1}{2}(P_x^2+\frac{\mathcal{E}_x^2}{X^2})+\frac{1}{2}(P_y^2+\frac{\mathcal{E}_y^2}{Y^2})+\frac{k}{2}(X^2-Y^2)-(K/2)\log(X+Y). \tag{4.75}$$

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 [23]. (Since the phase advance appears nowhere in the Hamiltonian, the emittance is constant, as expected). Taking this view, we obtain

$$\begin{aligned} \mu_x = &\quad \mathcal{E}_x \int \frac{dz}{X^2}, \\ \mu_y = &\quad \mathcal{E}_y \int \frac{dz}{Y^2}. \end{aligned} \tag{4.76}$$

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.

4.4 3D RMS Equations

In complete analogy to the previous section, we can also derive 3D rms envelope equations. Here we will consider a beamline consisting of rf gaps and quadrupoles. The single particle Hamiltonian was given in Eqs. (2.80) - (2.82), and the choice of scaling parameters (l, δ, ω) (to make the variables dimensionless) was given in Eqs. (2.80). Following Sacherer [20], one can obtain equations for the rms envelopes, X, Y and T:

$$X'' + \frac{p_o'}{p_o}X' + \frac{qg_m}{p_o}X - \frac{qg_{rf}}{p_o}X - \frac{\bar{K}u_o\pi\lambda_3}{l^2}XG_{311}(X,Y,u_oT) - (\frac{\delta}{lp_o})^2\frac{\mathcal{E}_{n,x}^2}{X^3} = 0,$$

$$Y'' + \frac{p_o'}{p_o}Y' - \frac{qg_m}{p_o}Y - \frac{qg_{rf}}{p_o}Y - \frac{\bar{K}u_o\pi\lambda_3}{l^2}YG_{131}(X,Y,u_oT) - (\frac{\delta}{lp_o})^2\frac{\mathcal{E}_{n,y}^2}{Y^3} = 0,$$

$$T'' + 3\frac{p_o'}{p_o}T' - \frac{q\omega_\alpha/c^2}{\gamma_o^2\beta_o^2p_o}e\sin\phi_sT - \frac{\bar{K}u_o\pi\lambda_3}{l^2}TG_{113}(X,Y,u_oT) - (\frac{\delta}{lp_ou_o^2})^2\frac{\mathcal{E}_{n,t}^2}{T^3} = 0, \tag{4.77}$$

where

$$g_{rf} = \frac{1}{2}[\frac{\omega_\alpha}{c^2}e\sin\phi_s - \frac{(\omega/\omega_\alpha)^2}{v_o}e'\cos\phi_s]. \tag{4.78}$$

In the above equations, $\mathcal{E}_{n,x}$, $\mathcal{E}_{n,y}$ and $\mathcal{E}_{n,t}$ denote normalized rms emittances. The quantity λ_3 is a geometrical factor that depends on the details of the charge distribution within the bunch, but as Sacherer pointed out it is not very sensitive to the details and has a value approximately equal to $1/(5\sqrt{5})$ for a wide variety of distributions. Lastly, the quantity G is a geometrical space charge term defined by

$$G_{mnp}(x,y,z) = \frac{3}{2}\int_0^\infty \frac{ds}{(x^2+s)^{m/2}(y^2+s)^{n/2}(z^2+s)^{p/2}}. \tag{4.79}$$

Note that these rms equations are *not* expected to accurately model the bunching process. The reason for this is twofold: (1) By our paraxial expansion of the single particle Hamiltonian, we assume that the external rf fields vary linearly across a bunch; (2) The space charge terms are based on the fields of an *isolated* bunch of charge, not a train of bunches.

Lastly, the rms equations are derivable from the following envelope Hamiltonian:

$$H^{\text{env}}(X,P_x,Y,P_y,T,P_t) = \frac{\delta}{2lp_o}(P_x^2+\frac{\mathcal{E}_{n,x}^2}{X^2}) + \frac{\delta}{2lp_o}(P_y^2+\frac{\mathcal{E}_{n,y}^2}{Y^2}) + \frac{\delta}{2lp_ou_o^2}(P_t^2+\frac{\mathcal{E}_{n,t}^2}{T^2})$$
$$+\frac{qlg_m}{2p_o}(X^2-Y^2) - \frac{qlg_{rf}}{2\delta}(X^2+Y^2) - \frac{q\omega_\alpha e\sin\phi_s}{2\omega^2 l\delta}T^2 + \frac{\bar{K}u_o^2\pi\lambda_3}{l}G_{111}(X,Y,u_oT) \tag{4.80}$$

4.5 RMS Matching with Contraction Map Techniques

4.5.1 2D Case

Consider a periodic transport system with period L. Let $\zeta = (X, P_x, Y, P_y)$. As shown above the envelope equations are derivable from a Hamiltonian; hence they define a symplectic nonlinear mapping $\mathcal{M}$ that maps initial state vectors into final state vectors:

$$\zeta^{\text{fin}} = \mathcal{M}\zeta^{\text{in}}. \tag{4.81}$$

If we consider transport through one period of the transport system, then a matched envelope is simply a fixed point of $\mathcal{M}$:

$$\mathcal{M}\zeta = \zeta. \tag{4.82}$$

Techniques for finding fixed points of symplectic maps are widely used in accelerator physics [10]. For example, they are used to find the off-momentum closed orbits of particles in circular machines. In our case, however, we will use the techniques to find the fixed points of an envelope map, not a particle map. The approach is based on the fact that the machinery exists to compute the action of the nonlinear map $\mathcal{M}$ as well as its linear part, M. This makes it easy to construct a contraction map based on a Newton search procedure to find the fixed point. As a result, the method is quadratically convergent. As an illustration, consider the problem of finding solutions of the equation $g(x) = x$, or equivalently, of finding roots of the function $f(x) = g(x) - x$. The Newton search algorithm defines a contraction mapping C that, for sufficiently close starting values, converges to a root [24]. If x^n is the value of x on the nth iteration, then applying the contraction map C to x^n produces a value at the next iteration:

$$x^{n+1} = Cx^n = x^n - \frac{f(x^n)}{f'(x^n)} = x^n - \frac{x^n - g(x^n)}{1 - g'(x^n)}. \tag{4.83}$$

It is easily shown that if x^n is within ϵ of a root then Cx^n deviates by an amount proportional to ϵ^2.

For a multidimensional system, the contraction map is given by [10]

$$\zeta^{n+1} = C\zeta^n = \zeta^n - (I - M)^{-1}(\zeta^n - \mathcal{M}\zeta^n), \tag{4.84}$$

where I is the identity matrix and M is the matrix associated with linear part of $\mathcal{M}$. To obtain M, first we need to linearize H^{env} about a "given" fiducial trajectory, ζ_g. Let $\hat{\zeta} = \zeta - \zeta_g$. The quadratic part of the Hamiltonian governing these deviation variables, which we will denote H_2, is given by

$$H_2 = \frac{1}{2}(\hat{P}_x^2 + \hat{P}_y^2) + \frac{\hat{X}^2}{2}[k + \frac{3\mathcal{E}_x^2}{X_g^4} + \frac{(K/2)}{(X_g + Y_g)^2}] + \frac{\hat{Y}^2}{2}[-k + \frac{3\mathcal{E}_y^2}{Y_g^4} + \frac{(K/2)}{(X_g + Y_g)^2}] + \frac{(K/2)\hat{X}\hat{Y}}{(X_g + Y_g)^2}. \tag{4.85}$$

As stated previously, M satisfies the equation

$$\frac{dM}{dz} = JSM, \tag{4.86}$$

where the symmetric matrix S is related to H_2 by

$$H_2(\hat{\zeta}, t) = \frac{1}{2} \sum_{a,b=1}^{4} S_{ab} \hat{\zeta}_a \hat{\zeta}_b. \tag{4.87}$$

Comparing Eq. (4.85) and Eq. (4.87) (with $\hat{\zeta} = (\hat{X}, \hat{P}_x, \hat{Y}, \hat{P}_y)$) one can immediately identify the matrix elements of S. That is, S_{11} is the coefficient of $\frac{1}{2}\hat{X}^2$, S_{22} is the coefficient of $\frac{1}{2}\hat{P}_x^2$, $S_{13} = S_{31}$ is the coefficient of $\hat{X}\hat{Y}$, *etc.*

Summarizing, Eq. (4.84) defines a contraction map for finding matched rms envelopes. In order to evaluate the right hand side of the equation, one must use numerical integration to compute the following: (1) $\mathcal{M}\zeta$, which is just the numerical solution of Hamilton's equations with the Hamiltonian of Eq. (4.75); and (2) the matrix M, which is obtained by numerically integrating $M' = JSM$. These quantities are computed at every iteration until the difference between $C\zeta$ and ζ is sufficiently small. For example, one might consider the map to have converged when $|\zeta - C\zeta|/|\zeta| < 10^{-8}$. One can use the zero current matched values as starting values for the contraction mapping procedure. For systems where these cannot be found analytically, we can begin by integrating the envelope equations with zero current and zero emittance; this is equivalent to computing the beta functions, from which we obtain the zero current matched envelopes.

4.5.2 3D Case

As in the two dimensional case, we need to compute the matrix M that describes the linear behavior of the system governed by H^{env}. This in turn requires that we know the matrix S, which appears in Eqs. (4.86) and (4.87). Linearizing H^{env} around a given fiducial trajectory ζ_g we obtain the following nonzero matrix elements of S:

$$S_{22} = S_{44} = \frac{\delta}{l p_o}, \quad S_{66} = \frac{\delta}{l p_o u_o^2}, \tag{4.88}$$

$$S_{11} = \frac{ql}{\delta}(g_m - g_{rf}) + \frac{\delta}{l p_o} \frac{3\mathcal{E}_{n,x}^2}{X_g^4} + \frac{\bar{K} u_o^2 \pi \lambda_3}{l}(3X_g^2 G_{511} - G_{311}), \tag{4.89}$$

$$S_{33} = \frac{ql}{\delta}(-g_m - g_{rf}) + \frac{\delta}{lp_o}\frac{3\mathcal{E}_{n,y}^2}{Y_g^4} + \frac{\bar{K}u_o^2\pi\lambda_3}{l}(3Y_g^2 G_{151} - G_{131}), \quad (4.90)$$

$$S_{55} = -\frac{q\omega_\alpha e \sin\phi_s}{\omega^2 l\delta} + \frac{\delta}{lp_o}\frac{3\mathcal{E}_{n,t}^2}{u_o^2 T_g^4} + \frac{\bar{K}u_o^4\pi\lambda_3}{l}(3u_o^2 T_g^2 G_{115} - G_{113}), \quad (4.91)$$

$$S_{13} = S_{31} = \frac{\bar{K}u_o^2\pi\lambda_3}{l} X_g Y_g G_{331}, \quad (4.92)$$

$$S_{15} = S_{51} = \frac{\bar{K}u_o^4\pi\lambda_3}{l} X_g T_g G_{313}, \quad (4.93)$$

$$S_{35} = S_{53} = \frac{\bar{K}u_o^4\pi\lambda_3}{l} Y_g T_g G_{133}. \quad (4.94)$$

Note that we have used the notation G_{mnp} to denote $G_{mnp}(X, Y, u_o T)$ in the above equations.

Chapter 5

Particle Simulation Techniques

5.1 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 subgrid 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 and solenoids in chapter 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, Eq. (2.11), 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

$$A_z^{self} = \frac{\beta_o}{c}\Psi^{self} \tag{5.1}$$

in MKSA units. Upon expanding Eq. (2.11), the two terms involving Ψ^{self} and A_z^{self} can be combined into a single term. The result, for a quadrupole system, is

$$H(\bar{x},\bar{p}_x,\bar{y},\bar{p}_y,z) = \frac{1}{2l}(\bar{p}_x^2+\bar{p}_y^2)+\frac{lk(z)}{2}(\bar{x}^2-\bar{y}^2)+\frac{K/2}{l}\hat{\Psi}(l\bar{x},l\bar{y},z), \tag{5.2}$$

where

$$k(z) = (q/p_o)g(z), \tag{5.3}$$

where K is the generalized perveance,

$$K = \frac{qI}{2\pi\epsilon_o p_o v_o^2\gamma_o^2}. \tag{5.4}$$

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

$$\Psi^{\text{self}} = \frac{\lambda}{4\pi\epsilon_o}\hat{\Psi}. \tag{5.5}$$

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.

- **Problem 5.1**
  For the quadupole system, expand the Hamiltonian, Eq. (2.11), assuming that the potentials come from externally applied fields given in Eq. (2.36) and self-fields Ψ^{self} and $\vec{A}_z^{self}$ that satisfy Eq. (5.1). Keep second order terms in x, p_x, y, p_y, and keep first order terms in Ψ^{self}, $\vec{A}_z^{self}$. Show that you obtain Eq. (5.2).

Similarly, for a solenoid system the Hamiltonian is

$$H(\bar{x},\bar{p}_x,\bar{y},\bar{p}_y,z) = \frac{1}{2l}(\bar{p}_x^2+\bar{p}_y^2)+l\frac{\alpha^2(z)}{2}(\bar{x}^2+\bar{y}^2)-\alpha(z)\,(\bar{x}\bar{p}_y-\bar{y}\bar{p}_x)+\frac{K/2}{l}\hat{\Psi}(l\bar{x},l\bar{y},z), \tag{5.6}$$

where

$$\alpha(z) = \frac{qB_o}{2p_o}. \tag{5.7}$$

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:

$$H = H_{ext} + H_{self} \tag{5.8}$$

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

$$H_{self} = \frac{K}{2}\hat{\Psi}(x,y). \tag{5.9}$$

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

$$\begin{aligned} x^{fin} &= x^{in}, \\ p_x^{fin} &= p_x^{in} - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial x}, \\ y^{fin} &= y^{in}, \\ p_y^{fin} &= p_y^{in} - \frac{K}{2}\frac{\partial\hat{\Psi}}{\partial y}. \end{aligned} \tag{5.10}$$

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. But for round beams this is easily accomplished, as described in the following section.

5.2 Simulation of Round Beams

When treating long beams (as opposed to bunched beams) it is conventional to treat the problem as a two-dimensional problem; thus, even though the beam profile changes along the transport system, the fields are often computed at a given location z is if the beam profile present at that location extended to plus and minus infinity. Poisson's equation reduces to a two-dimensional problem,

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = \rho/\epsilon_o. \tag{5.11}$$

In later sections we will deal with the solution of this problem using Particle-In-Cell (PIC) techniques. However, if the beam is round the problem becomes very easy to deal with. We start with Gauss' law,

$$\int \vec{E}\cdot d\vec{S} = \frac{Q_{encl}}{\epsilon_o}, \tag{5.12}$$

where Q_{encl} is the charge enclosed in the cylindrical surface S. In free space the electric field will be radial with respect to the centroid, and

we obtain

$$2\pi r E_r = \frac{\lambda}{\epsilon_o}\int^r 2\pi r' n(r')\, dr', \tag{5.13}$$

where $n(r)$ is the number density, where λ is the charge per unit length. The integral in the above equation is equal to the fraction of charge inside a cylinder of radius r. It follows that, in a simulation of a round beam with N particles, the radial electric field experienced by the kth particle, located at radius r_k, is given by

$$E_r(r_k) = \frac{\lambda}{2\pi r_k \epsilon_o} F_k, \tag{5.14}$$

where

$$F_k = \frac{1}{N} \times rank\ of\ the\ kth\ particle, \tag{5.15}$$

where, by rank, we mean the ranking in radius of the kth particle. Thus, all that is needed to compute the self-fields in a round beam simulation is a routine to order particles based on their radii. Such an ordering routine can be found in many texts on numerical methods, an in addition such a routine is standard in High Performance Fortran.

The key subroutines for a split-operator code for round beams in a solenoid channel is shown below. The routine `map1` corresponds to H_{ext}, and `map2` corresponds to H_{self}. Subroutine `spchg` is small and could of course be put directly inside `map2`, but we have written a separate routine since this is the structure of the code that will be used when we treat more general beams without cylindrical symmetry.

```
      subroutine map1(z,tau,y,yt)
! linear map for an idealize solenoid
      implicit real(a-h,o-z)
      parameter(np=1000000)
      dimension y(4,np),yt(4,np)
      common/solen/b0,alph
!hpf$ distribute y(*,block)
!hpf$ align (*,:) with y(*,:) :: yt
      if(b0.eq.0.)then
        yt(1,:)=y(1,:)+tau*y(2,:)
        yt(2,:)=y(2,:)
```

```
        yt(3,:)=y(3,:)+tau*y(4,:)
        yt(4,:)=y(4,:)
      else
        cosat=cos(alph*tau)
        sinat=sin(alph*tau)
        yt(1,:)=      y(1,:)*cosat + y(2,:)*sinat/alph
        yt(2,:)=-alph*y(1,:)*sinat + y(2,:)*cosat
        yt(3,:)=      y(3,:)*cosat + y(4,:)*sinat/alph
        yt(4,:)=-alph*y(3,:)*sinat + y(4,:)*cosat
      endif
      z=z+tau
      return
      end

      subroutine map2(z,tau,y,yt)
! map for space charge kick
      implicit real(a-h,o-z)
      parameter(np=1000000)
      dimension y(4,np),yt(4,np),ex(np),ey(np)
      common/beamp/brho,perv
!hpf$ distribute y(*,block)
!hpf$ align (*,:) with y(*,:) :: yt
!hpf$ align (:) with y(*,:) :: ex,ey
      call spchg(y,ex,ey)
      pcon=0.5*perv/np
      ex=ex*pcon
      ey=ey*pcon
      yt(1,:)=y(1,:)
      yt(2,:)=y(2,:)+tau*ex
      yt(3,:)=y(3,:)
      yt(4,:)=y(4,:)+tau*ey
      return
      end

      subroutine spchg(y,ex,ey)
! Gauss' Law space charge routine for long, round beams.
! Units, normalization: d^2 phi/ dx^2 +d^2 phi /dy^2 =-rho, (no epsilon_o)
```

```
! where the volume integral of rho = 1.
      use hpf_library
      implicit real(a-h,o-z)
      parameter(np=1000000)
      dimension y(4,np),ex(np),ey(np),rr(np),jdest(np),nout(np)
      common/beamp/brho,perv
!hpf$ distribute y(*,block)
!hpf$ align (:) with y(*,:) :: ex,ey,rr,jdest,nout
      rr=y(1,:)**2+y(3,:)**2
      nout=grade_up(rr,1)
      forall(i=1:np)jdest(nout(i))=i
      jdest=jdest-1
      ex=jdest*y(1,:)/rr
      ey=jdest*y(3,:)/rr
      return
      end
```

5.3 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 [26] [27].

5.3.1 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. The routines `depngp2` and `intngp2`, for 2D, NGP charge deposition and field interpolation, are shown below.

```
      subroutine depngp2(y,rho)
! charge deposition on a 2D grid using NGP scheme
      implicit real(a-h,o-z)
      parameter(np=1000000,nx=64,ny=64)
      dimension y(4,np),rho(nx,ny),indx(np),jndx(np)
      common/gridp/hx,hy,hxi,hyi,xmin,ymin
!hpf$ distribute y(*,block)
!hpf$ align (:) with y(*,:) :: indx,jndx
!hpf$ distribute rho(*,block)
      indx=nint((y(1,:)-xmin)*hxi)
      jndx=nint((y(3,:)-ymin)*hyi)
      rho=0.
      do n=1,np
        rho(indx(n),jndx(n))=rho(indx(n),jndx(n))+1.0
      enddo
      return
      end
```

```
      subroutine intngp2(y,rho,exg,eyg,exg,eyg,indx,jndx)
! field interpolation on a 2D grid using NGP scheme
      implicit real(a-h,o-z)
      parameter(np=1000000,nx=64,ny=64)
      dimension y(4,np),ex(np),ey(np),indx(np),jndx(np)
      dimension rho(nx,ny),exg(nx,ny),eyg(nx,ny)
      common/gridp/hx,hy,hxi,hyi,xmin,ymin
!hpf$ distribute y(*,block)
!hpf$ align (:) with y(*,:) :: ex,ey,indx,jndx
!hpf$ distribute rho(*,block)
      do n=1,np
        ex(n)=exg(indx(n),jndx(n))
        ey(n)=eyg(indx(n),jndx(n))
      enddo
      return
      end
```

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. The routines `depcic2` and `intcic2`, for 2D, CIC charge deposition and field interpolation, are shown below.

```
      subroutine depcic2(y,rho)
! charge deposition on a 2D grid using CIC scheme
      implicit real(a-h,o-z)
      parameter(np=1000000,nx=64,ny=64)
      dimension y(4,np),rho(nx,ny),indx(np),jndx(np),ab(np),cd(np)
      common/gridp/hx,hy,hxi,hyi,xmin,ymin
!hpf$ distribute y(*,block)
!hpf$ align (:) with y(*,:) :: indx,jndx,ab,cd
!hpf$ distribute rho(*,block)
      indx=(y(1,:)-xmin)*hxi
```

```
      jndx=(y(3,:)-ymin)*hyi
      rho=0.
      ab=xmin-y(1,:)+indx*hx
      cd=ymin-y(3,:)+jndx*hy
      do n=1,np
       rho(indx(n),jndx(n))=rho(indx(n),jndx(n))+ab(n)*cd(n)
       rho(indx(n)+1,jndx(n))=rho(indx(n)+1,jndx(n))+cd(n)*(hx-ab(n))
       rho(indx(n),jndx(n)+1)=rho(indx(n),jndx(n)+1)+ab(n)*(hy-cd(n))
       rho(indx(n)+1,jndx(n)+1)=rho(indx(n)+1,jndx(n)+1)+(hx-ab(n))*(hy-cd(n))
      enddo
      return
      end



      subroutine intcic2(y,rho,exg,eyg,exg,eyg,indx,jndx,ab,de)
! field interpolation on a 2D grid using CIC scheme
      implicit real(a-h,o-z)
      parameter(np=1000000,nx=64,ny=64)
      dimension y(4,np),ex(np),ey(np),indx(np),jndx(np),ab(np),cd(np)
      dimension rho(nx,ny),exg(nx,ny),eyg(nx,ny)
      common/gridp/hx,hy,hxi,hyi,xmin,ymin
!hpf$ distribute y(*,block)
!hpf$ align (:) with y(*,:) :: ex,ey,indx,jndx,ab,cd
!hpf$ distribute rho(*,block)
      do n=1,np
        ex(n)=exg(indx(n),jndx(n))*ab(n)*cd(n)+
              exg(indx(n)+1,jndx(n))*cd(n)*(hx-ab(n))+
              exg(indx(n),jndx(n)+1)*ab(n)*(hy-cd(n))+
              exg(indx(n)+1,jndx(n)+1)*(hx-ab(n))*(hy-cd(n))
        ey(n)=eyg(indx(n),jndx(n))*ab(n)*cd(n)+
              eyg(indx(n)+1,jndx(n))*cd(n)*(hx-ab(n))+
              eyg(indx(n),jndx(n)+1)*ab(n)*(hy-cd(n))+
              eyg(indx(n)+1,jndx(n)+1)*(hx-ab(n))*(hy-cd(n))
      enddo
      return
      end
```

5.3.2 Solution of the Field Equations

5.3.3 Isolated Systems

Hockney's convolution algorithm for calculating the potential of isolated systems is described in [26]. 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

$$Y_l = \sum_{n=0}^{N-1} h_n X_{l-n} \qquad l = 0, \ldots, N-1 \tag{5.16}$$

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

$$\psi(\vec{x}) = \int d\vec{x}' \; \rho(\vec{x}) \; G(\vec{x} - \vec{x}'). \tag{5.17}$$

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. (5.16) 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. (5.16) by a circular convolution that matches (5.16) 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,

$$h_n = 0 \qquad \frac{N}{2} \leq n \leq N-1. \tag{5.18}$$

Define a periodic Green function χ_l, by

$$\begin{aligned} \chi_l &= X_l \qquad -\frac{N}{2} \le l \le \frac{N}{2} - 1, \\ \chi_{l+N} &= \chi_l. \end{aligned} \tag{5.19}$$

Now consider the sum

$$\hat{Y}_l = \frac{1}{N} \sum_{k=0}^{N-1} W^{-lk} (\sum_{n=0}^{N-1} h_n W^{nk})(\sum_{m=0}^{N-1} \chi_m W^{mk}) \qquad 0 \le l \le N-1, \tag{5.20}$$

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

$$\hat{Y}_l = Y_l \qquad 0 \le l \le \frac{N}{2} - 1. \tag{5.21}$$

Proof: By Eq. (5.18)

$$\hat{Y}_l = \sum_{n=0}^{N/2-1} \sum_{m=0}^{N-1} h_n \chi_m \frac{1}{N} \sum_{k=0}^{N-1} W^{(m+n-l)k}. \tag{5.22}$$

Now use the relation

$$\sum_{k=0}^{N-1} W^{(m+n-l)k} = N \delta_{m+n,l+jN} \qquad (j \text{ an integer}). \tag{5.23}$$

It follows that

$$\hat{Y}_l = \sum_{n=0}^{N/2-1} h_n \ \chi_{l-n+jN}. \tag{5.24}$$

But χ is periodic with period N. Thus,

$$\hat{Y}_l = \sum_{n=0}^{N/2-1} h_n \, \chi_{l-n} = \sum_{n=0}^{N/2-1} h_n \, X_{l-n} \quad \text{if} \quad -\frac{N}{2} \le l-n \le \frac{N}{2}-1 \tag{5.25}$$

That is,

$$\hat{Y}_l = Y_l \tag{5.26}$$

if

$$-\frac{N}{2} + n \le l \le \frac{N}{2} - 1 + n \tag{5.27}$$

and, from Eq. (5.25),

$$0 \leq n \leq N/2 - 1. \tag{5.28}$$

But Eqs. (5.27) and (5.28) are clearly satisfied for

$$0 \leq l \leq N/2 - 1, \tag{5.29}$$

so the proof is complete.