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Benchmarks in Numerical Methods

for single particle trajectories

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Accelerated charges emit radiation. This fundamental idea in plasma physics has deep consequences in the design of particle accelerators and radiation sources, who have together many important applications in the present time. I will address this issue by looking at very basic field configuration and present a detailed argumentation, from the Maxwell equations to the trajectories, radiation spectra and other results.

1 Contents

2 Introduction

This text is a collection of notes organised to help clarify the work done during these six months at GoLP - Group of Lasers and Plasmas, a subdivision of IPFN - Instituto de Plasmas e Fusão Nuclear (Institute of Plasmas and Nuclear Fusion), specialized in extreme plasma-laser interactions.
The initial internship benchmarks can be sumarized as follows:

– 1) Individual particle and counter propagating laser: first harmonics as functions of a_0 and w_0 , with $a_0 w_0 = cte$, that is, how does the radiation spectrum change even if the energy is constant.

– 2) Can individual particles and plasmas in magnetic bottles be used as radiation sources?

– 3) What are the radiation spectra of individual particles and plasma in magnetic dipoles and how can they be deduced by the plasma properties.Further comments

Chapter 1: Notes on method stability

2.1 Normalization

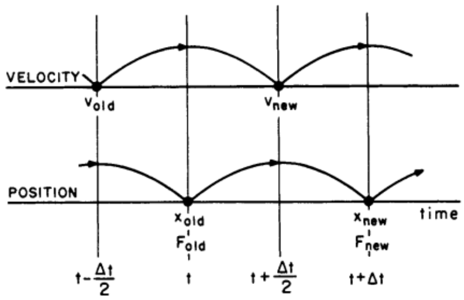
Because simulation values of interest can become extremely small or large, normalization of the variables is standard procedure. We take:

$$\begin{aligned} t &\to \hat{t} = \omega t \\ \mathbf{x} &\to \hat{\mathbf{x}} = kx \\ \mathbf{v} &\to \hat{\mathbf{v}} = v/c \\ \mathbf{p} &\to \hat{\mathbf{p}} = p/(mc) \\ \mathbf{A} &\to \hat{\mathbf{A}} = e\mathbf{A}/(mc^2) \\ \mathbf{E} &\to \hat{\mathbf{E}} = e\mathbf{E}/(m\omega c), \\ \mathbf{B} &\to \hat{\mathbf{B}} = e\mathbf{B}/(m\omega c) \end{aligned}$$

with $\omega = k = c = e = m = 1$ (from [2]). A "hat" symbol implies that the variable is normalized, but from now on all equations will be written in a normalized way, implicitly. Numerical solutions must be used in order to probe deeper into physics in general, and into plasma physics in particular. Numerical errors can come from multiple sources: the stability of the method and the numerical precision of the machine. Unstable methods will always be associated with larger errors in the long run, whatever the numerical precision of the machine.

2.2 Leapfrog method

To problems solved in this context only require the knowledge of the pair coordinates/momenta and the forces acting on the particle at some instant. In ordinary methods, velocities and position are solved for the same instant. However, one soon realizes that another more natural process of calculation is needed. A method where the velocities are calculated $\Delta t/2$ before the position is called a Leapfrog method. We define $t^n = n \cdot \Delta t$ and ε as the electric field.



We now introduce one of the most common Leapfrog methods used in plasma physics: the Boris pusher (see [1] for the original deduction and picture). First we define $u = \gamma v$. As usual, the momentum change can be written as $(u^{n+1/2} - u^{n-1/2})/\Delta t$. But because we are using the momentum at time n to calculate the Lorentz force, one should use an average $(u^{n+1/2} + u^{n-1/2})/2$. Thus we get the differential equation $(u^{n+1/2} - u^{n-1/2})/\Delta t = q/m(\varepsilon^n + (u^{n+1/2} + u^{n-1/2})/(2c\gamma^n) \times B^n)$ (cgs units). By defining the auxiliary velocities $u^{n-1/2} = u^- - q\varepsilon^n \Delta t/(2 \cdot m)$ and $u^{n+1/2} = u^+ + qE\Delta t/(2m)$ and substituting in the Lorentz force equation we get $(u^+ - u^-)/\Delta t = q(u^+ + u^-) \times B^n/(2mc\gamma^n)$. As the article by Boris (1970) pointed out, this is equivalent to three ordered steps: a first ε-impulse, a B-rotation of u and a second ε-impulse. We add the intermediary momenta $u' = u^- + u^- \times t$ and $u^+ = u^- + u' \times s$ with $t = q\Delta t B/(2\gamma^n(u_1)mc)$ and $s = 2t/(||t||^2 + 1)$. The last step is to update the position by the simple equation $x^{n+1} = x^n + u^{n+1/2}/(\gamma^{n+1/2})$.

Consult the Appendix to see the basic form of the code.

2.3 Uniform $\varepsilon \parallel v0$

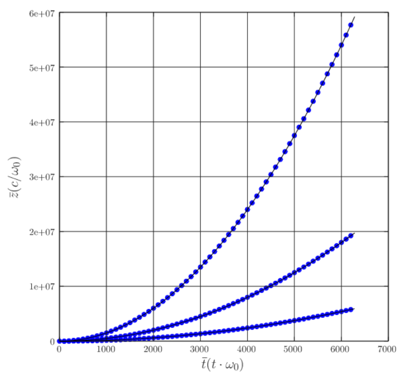
We now focus on elementary cases of particle motion. The next three sections can be skipped without loss of clarity.

Non-relativistic case

The common equation of motion becomes

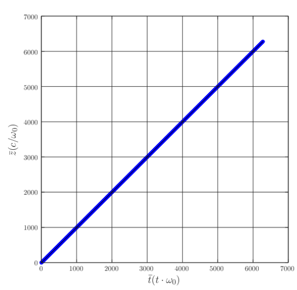
$$d\mathbf{p}/dt = d(m\mathbf{v})/dt = q\varepsilon e_z$$
$$x_0 = 0, v_0 = 0$$
$$\Longrightarrow$$
$$z(t) = q\varepsilon t^2/(2m)$$
$$\Longrightarrow^{(norm)}$$
$$z(t) = \varepsilon\ t^2/2$$

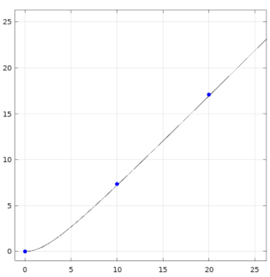
As expected, the progression of the z coordinate is a parabola in time. The values of ε associated with the curves are 0.3, 1.0 and 3.0, counting from the bottom of the plot to the top.



Relativistic case

$$dp/dt = d(\gamma\ m\ v)/dt = q\ \varepsilon\ e_z$$
$$x_0 = 0, v_0 = 0$$
$$\Longrightarrow (normalization)$$
$$z(t) = (\sqrt{(1 + (\varepsilon\ t)^2)} - 1)/\varepsilon$$





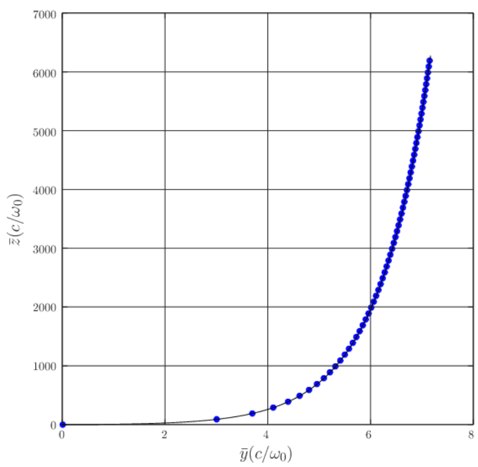
As expected the path is asymptotically a straight line of angle 45º (for the velocity cannot surpass c=1). However, by looking at the origin of the plot, we see a curve that is close to a parabola, because the two solutions are the same in the first Taylor expansion terms. As parameters we used $x_0 = 0, v_0 = 0.1e_y$, $\varepsilon = 0.1e_z$ and $\Delta t = 0.1$.

2.4 UNIFORM $\varepsilon \perp v_0$

Non-relativistic case
Starting with the initial value problem we get almost the same result as before.

$$\begin{aligned} dp/dt = d(m\ v)/dt = q\ \varepsilon e_z \\ x_0 = 0, v_0 = v_{0y} \\ \Longrightarrow (normalization) \\ z(t) = \varepsilon\ t^2/2 \\ y(t) = v_{0y}\ t \\ z(y) = y^2\ \varepsilon/(2\ v_{0y}^2) \end{aligned}$$

As parameters we used $x_0 = 0, v_0 = 0.9e_y, \varepsilon = 0.1e_z$ and $\Delta t = 0.1$.



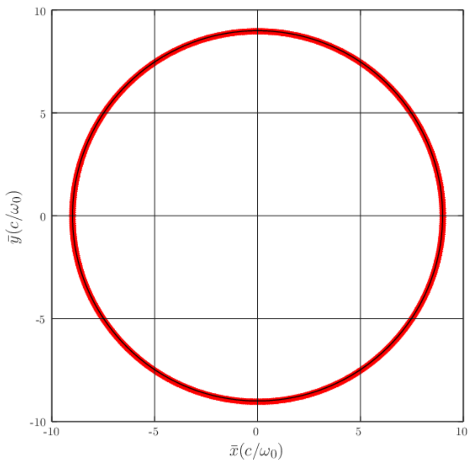
2.5 UNIFORM B $\perp$ V

In previous cases we have only looked at the electric field and set the magnetic field to zero. We now invert the roles of the fields and study the case of cyclotron/synchrotron motion.

Relativistic case

$$\begin{aligned} dp/dt = d(\gamma\ v)/dt = -[vxB]e_z \\ x_0 = Rex, v_0 = v_0 ey \\ R = vo/\omega = vo\ \gamma_0/B \\ \Longrightarrow \\ x(t) = R\ cos(\omega\ t) \\ y(t) = R\ sin(\omega\ t) \end{aligned}$$

As parameters we used $x_0 = Re_x, v_0 = 0.9e_y, B = 0.1e_z$ and $\Delta t = 0.1$.



CHAPTER 2: NOTES ON PLANE WAVE INTERACTION

2.6 EM-FIELD EQUATIONS

In this section we present the field equations as is done in 1. This part can be skipped without loss of clarity. In our first configuration, a plane wave $A = (0, \delta a_0 \cos\phi, (1-\delta^2)^{1/2} a_0 \sin\phi)$ travels in the positive x direction towards an electron, where $\phi = \omega t - k \cdot x$.
By choosing a linear polarization $\delta = 1$ and using

$$\begin{aligned} E = -\partial A/\partial t \\ B = \nabla \times A = (0, -\partial A_z/\partial x, \partial A_y/\partial x) \end{aligned}$$

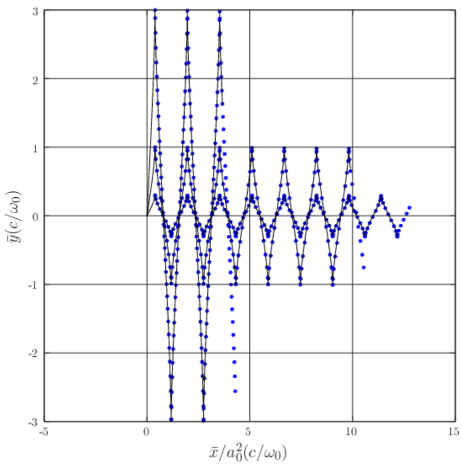
the EM-field equations become (see Appendix)

$$\begin{aligned} E = \omega\ a_0\ sin(\omega \cdot t - k \cdot x - \phi_0)\ f(t) \cdot e_y \\ B = k \cdot a_0 \cdot sin(\omega \cdot t - k \cdot x - \phi_0) \cdot f(t) \cdot e_z \end{aligned}$$

where f(t) is an envelope function that mimics the "package" nature of the wave. When needed, we shall take a "ramp-like" function that grows linearly in some interval T_0 and takes the value 1 in further instants.

2.7 Figure-of-eight

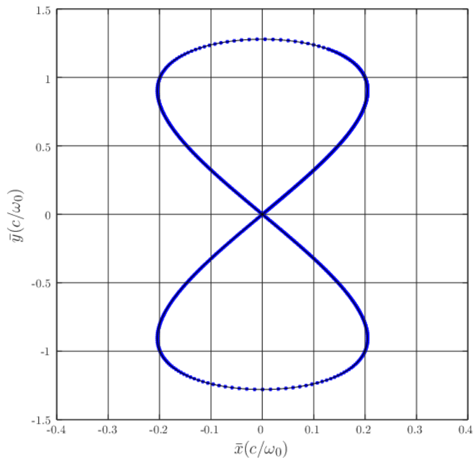
For linear polarization we have $x = 0.125 a_0^2 sin(2\phi)$ and $y = a_0 sin(\phi)$ Indeed, the result is coincident with the predicted analytical solution. No envelope function was used and the effect of radiation friction was neglected. The time step used was 0.001 and a_0 is of values of 0.3, 1 and 3.0, corresponding to the smallest to the largest figure.



A secular motion is present, according to a velocity of $v_D = a_0^2/(4+a_0^2)$ in the x direction. To "eliminate" this motion we apply a simple Lorentz transformation $x'(t) = \gamma(v_D)(x(t) - v_D t)$, that is, the motion in a frame of reference (which we call "rest" frame), which has the velocity v_D in the "lab" frame. The general transformation can be represented as a matrix Λ, which is to be multiplied by the four-vector (ct, x^1, x^2, x^3). In this case, $\gamma = \gamma(v_D)$, which is constant over time.

$$\begin{cases} \vec{\mathbf{r}}'_{\parallel} = \gamma(\vec{\mathbf{r}}_{\parallel} - vt) \\ \vec{\mathbf{r}}'_{\perp} = \vec{\mathbf{r}}_{\perp} \\ t' = \gamma \cdot (t - (\vec{r} \cdot \vec{v})/c^2) \end{cases} \tag{2.1}$$

Having applied the transformation, one gets the common motion of "figure-of-eight". In particular, in the plot shown below $a_0 = 3.0$. A scaling of $x \to x/\gamma_0$, with $\gamma_0 = \sqrt{1 + 0.5 a_0^2}$.



2.8 Comments

A great deal of difficulty was present in trying to get the figure of eight of the electron motion. However, a simple matrix multiplication of Λ by the four-vector (ct, x^1, x^2, x^3) for each iteration should do the job.

~~There is a pathological inconsistency with the equations of motion, for the initial energy is zero, and for the motion to become fully periodic, it would have to start with the momentum it would have had it started the motion some periods before. Because of this~~, the particle was injected with the momentum it would have in the figure of eight, and no phase shift was needed in the equations of motion.

2.9 Radiation spectrum

We now draw our attention to the "classical" radiation of the charge. This is an obvious approximation, because a continuously emitting charge will loose energy over time. Such processes are not accounted here. As in the previous chapter, we analyze example by example.

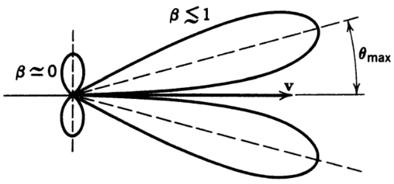
The general formula for radiated power by solid angle is (see [Jackson])

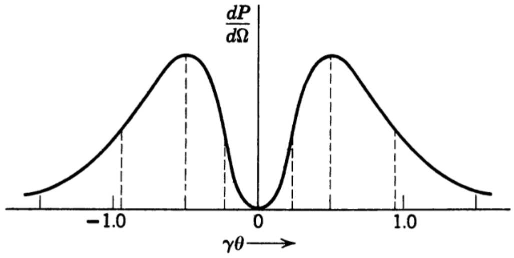
$$\frac{dP(t')}{d\Omega} = \frac{1}{4\pi} \frac{[\vec{n} \times [(\vec{n} - \vec{v}) \times \dot{\vec{v}}]]}{(1 - \vec{n} \cdot \vec{v})^5} \tag{2.2}$$

2.10 UNIFORM E ∥ V

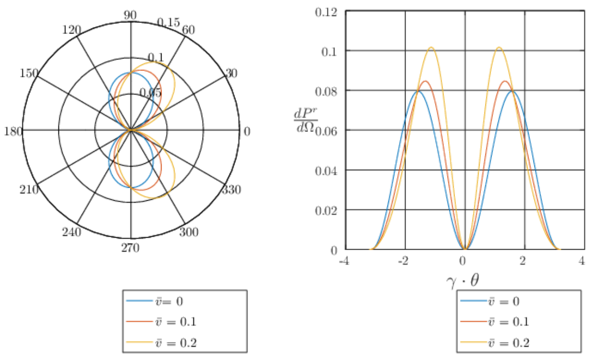
$$\frac{dP(t')}{d\Omega} = \frac{e^2 \dot{v}^2}{4\pi c^3} \frac{\sin^2\theta}{(1 - \beta cos\theta)^5} \tag{2.3}$$

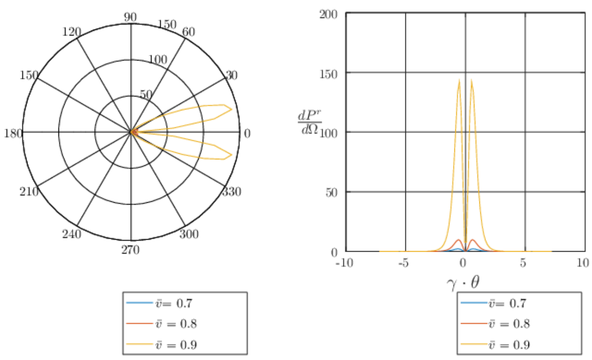
According to Jackson





Below to the left is a polar plot representing the power as a function of the observation angle given by the expression 2.3 and a plot to the right showing the same information in a Cartesian way. It resembles the image of a headlight, with an ever decreasing θ_{max} when $v \approx c$.

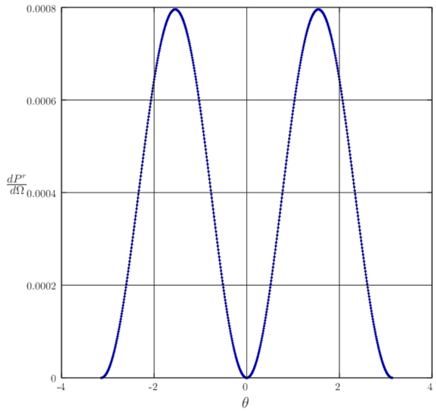




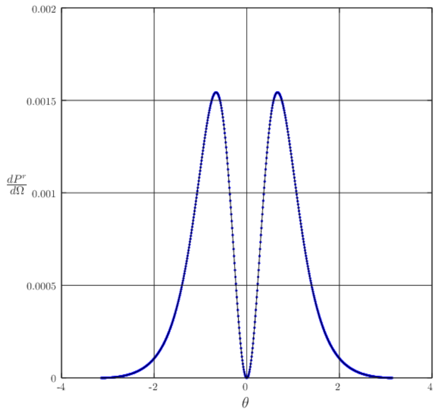
If we plot $dP/d\Omega$ as a function of θ, we should get a symmetric two-peak function, with both peaks closer to $\theta = 0$ when $v/c \approx 1$.

Adapting the general code for a constant electric field, the simulation gives the following plots for specific velocities sampled in time.

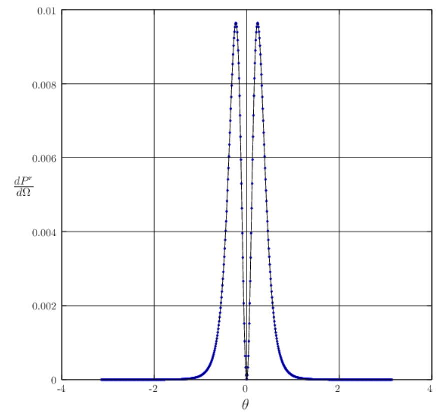
v/c=0.1



v/c=0.5



v/c=0.9



2.11 UNIFORM B $\perp$ V

We choose a geometry in which we can choose the observation angle in relation to the velocity and acceleration.

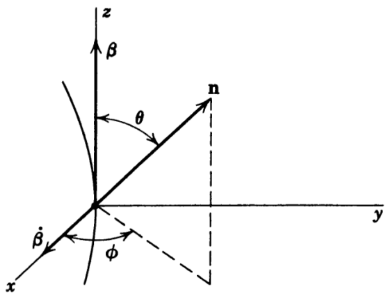
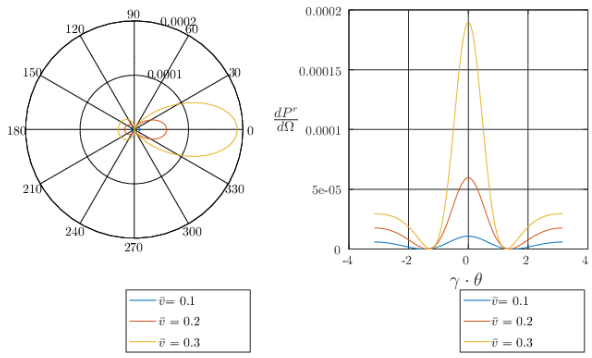


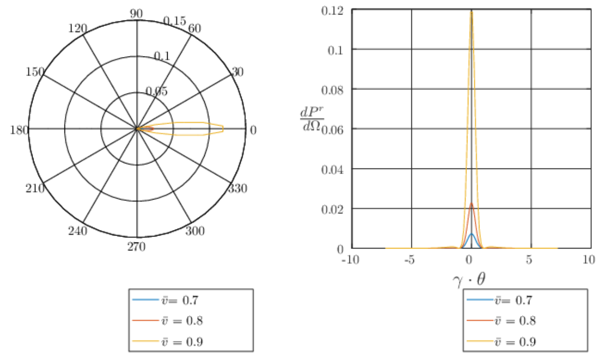
Image taken from [Jackson]

In the case of circular motion, the power spectrum becomes:

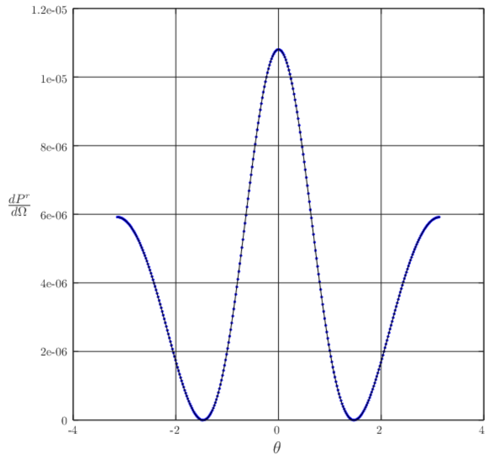
$$\frac{dP(t')}{d\Omega} = \frac{e^2}{4\pi c^3} \frac{\dot{v}^2}{(1-\beta cos\theta)^3} \left[1 - \frac{\sin^2\theta \cos^2\phi}{\gamma^2 (1-\beta cos\theta)^2} \right] \tag{2.4}$$

Now, the polar plot clearly indicates that for low velocities the spectrum resembles that of a magnetic dipole ???, but looses this symmetry when $v \approx c$.

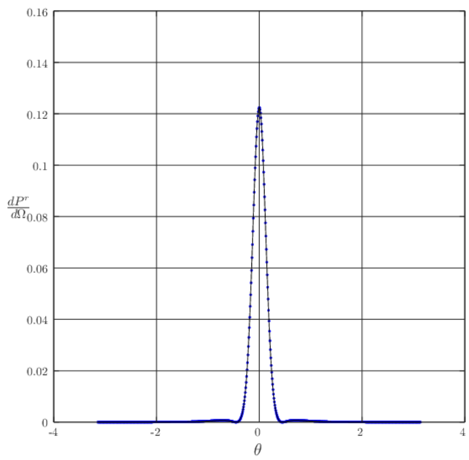




v/c=0.1



v/c=0.9



The relation between intensity and power by solid angle is:

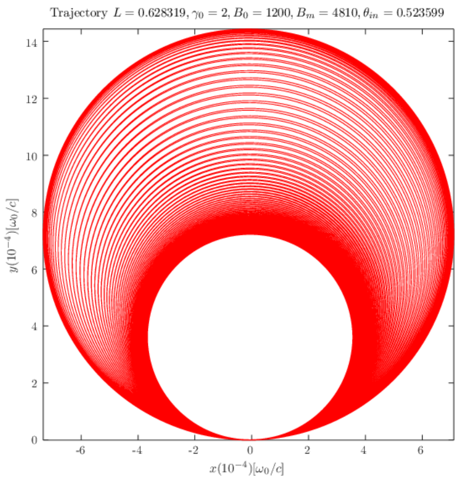
$$\frac{dP_m}{d\Omega} = \frac{\omega_0^2}{2\pi} \frac{d^2 I}{d\omega d\Omega} \tag{2.5}$$

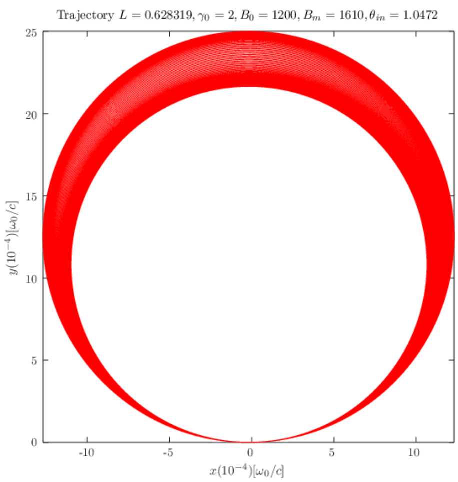
$$\frac{dP_m}{d\Omega} = \frac{\omega_0^2}{2\pi} \frac{d^2 I}{d\omega d\Omega} \tag{2.6}$$

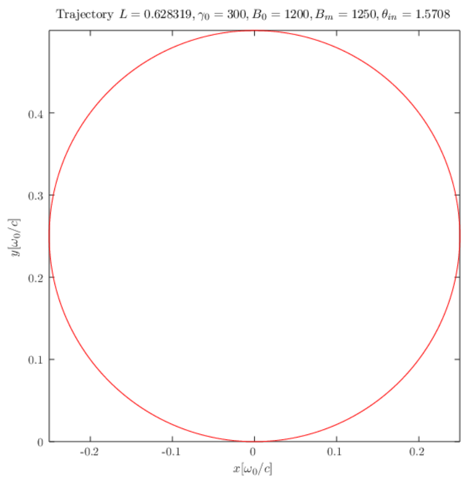
CHAPTER 4: NOTES ON "MAGNETIC BOTTLES"

A "magnetic mirror" is a configuration of the magnetic field that confines particles with certain initial conditions to a limited region of space. We call B_m the maximum B field intensity, and B_0 the minimum value. Particles with an injection angle less than the critical angle θ_c will eventually escape the region. This parameter is given by the expression $\theta_c = \sqrt{\arcsin(B_0/B_m)}$.

L is the reference parameter for the size of the confinement region. $B_z(z) = B_m - (B_m - B_0)exp(-(\frac{z-0.9L}{0.7L})^1 2)$







Holkandkar
The loss cone.

MAGNETIC TRAP: EXAMPLE 1

MAGNETIC TRAP: EXAMPLE 2

MAGNETIC CUSP

CHAPTER 5: NOTES ON MAGNETIC DIPOLES

APPENDIX A: CODE

For convenience, we rename the variables as follows:

$$u^- \to u_1, u' \to u_2, u^+ \to u_3$$

We also define two ways of calculating the gamma factor: $\gamma_1 = 1/\sqrt{(}1-v^2)$ and $\gamma_2 = \sqrt{(}1+u^2)$. The first will only be used (at most) when defining the initial conditions (setting a particular v/c), but the algorithm will always work with the second definition, so we will assume this will be the calculation made whenever a γ factor arises. Furthermore, the second method also avoids the numerical complications of the first (in the case $v \approx c$. We now present an Octave version of the code, which will be the skeleton for all the applications written for this paper.

```
#"Push" back half step
     t=0;
     #getFields
     F=getFields(dt,t,x,u,a0,w0);
     Ex=-F(1,:);
     Bx=-F(2,:);
     #auxiliary rotation variables
     auxt=qm*dt2*Bx/gamma2(u);
     auxs=2*auxt/(norm(auxt)*norm(auxt)+1);
```

```
    #half rotation
    u2=u+cross(u,auxt);
    u3=u+cross(u2,auxs);
    #half E-impulse
    u=u3+qm*dt2*Ex;

while( t<titer)
    #getFields
        F=getFields(dt,t,x,u,a0,w0);
        Ex=F(1,:);
        Bx=F(2,:);

    #first E-impulse
        u1=u(1,:)+qm*dt2*Ex;

    #auxiliary rotation variables
    auxt=qm*dt2*Bx/gamma2(u1);
    auxs=2*auxt/(norm(auxt)*norm(auxt)+1);

    # rotation
        u2=u1+cross(u1,auxt);
        u3=u1+cross(u2,auxs);

    #second E-impulse
        u=u3+qm*dt2*Ex;

    #gamma
        gm0=gamma2(u);

    #x
        x(1,:)+=dt*u/gm0;

    #save iterations
        vecTl(t+1,:)=t*dt;
        vecXl(t+1,:)=x(1,:);
        vecUl(t+1,:)=u(1,:);
    #inc tempo
    t++;
endwhile
```

where qm = q/m = -1 (for electrons), dt2 = dt/2.

We often need to transform coordinates from one inertial frame of reference (FR) to another. The code that was used for this task is a simple matrix multiplication, as shown below.

```
#Frame of Reference velocity components
    b1=vecFR(1,1);
    b2=vecFR(1,2);
    b3=vecFR(1,3);
    bsq=b1^2+b2^2+b3^3; # the norm squared
    gm=gamma1(vecFR); # the FR's relative
gamma
    matLB=zeros(4,4);
    matSr=zeros(4,1);

    matLB = [
gm, -gm*b1, -gm*b2, -gm*b3 ,
gm*b1, 1+(gm-1)*b1*b1/bsq,
(gm-1)*b2*b1/bsq, (gm-1)*b3*b1/bsq,
gm*b2, (gm-1)*b1*b2/bsq,
1+(gm-1)*b2*b2/bsq, (gm-1)*b3*b2/bsq,
gm*b3, (gm-1)*b1*b3/bsq,
(gm-1)*b2*b3/bsq, 1+(gm-1)*b3*b3/bsq
]; # Lorentz boost matrix

# Apply Boost to old Reference Frame (S)
    for(t=1:titer)
        matSr = matLB*[vecTl(t),vecXl(t,1),vecXl(t,2
        vecTr(t,1)=matSr(1);
        vecXr(t,1)=matSr(2);
        vecXr(t,2)=matSr(3);
        vecXr(t,3)=matSr(4);
    endfor
```

LORENTZ BOOST

$$\Lambda = \begin{pmatrix} \gamma & -\gamma\beta^1 & -\gamma\beta^2 & -\gamma\beta^3 \\ \gamma\beta^1 & 1+(\gamma-1)(\beta^1)^2/|\beta|^2 & (\gamma-1)\beta^2\beta^1/|\beta|^2 & (\gamma-1)\beta^3\beta^1/|\beta|^2 \\ \gamma\beta^2 & (\gamma-1)\beta^1\beta^2/\beta^2 & 1+(\gamma-1)(\beta^2)^2/|\beta|^2 & (\gamma-1)\beta^3\beta^2/\beta^2 \\ \gamma\beta^3 & (\gamma-1)\beta^1\beta^3/\beta^2 & (\gamma-1)\beta^2\beta^3/\beta^2 & 1+(\gamma-1)(\beta^3)^2/|\beta|^2 \end{pmatrix} \quad (2.7)$$

EQUATIONS OF MOTION FOR THE PLANE WAVE INTERACTION

Here we follow the steps of [Gibbon] in the deduction of the equations of motion. The laser EM vector potential can be described as

$$\vec{A} = (0, A, 0) = (0, a_0 cos(\phi), 0) \quad (2.8)$$

where we have chosen a simple linear polarization. We then have

$$\vec{E} = -\partial\vec{A}/\partial t = (0, \omega_0 a_0 sin(\phi), 0) \quad (2.9)$$

and

$$\begin{aligned} \vec{B} = \nabla\times\vec{A} = (0, \partial A_z/\partial x, \partial A_y/\partial x) = \\ = (0, 0, -k\cdot a_0\cdot sin(\phi)) \end{aligned} \quad (2.10)$$

Now that we have the fields, we can write Newton's equation

$$d\vec{p}/dt = -e\cdot(\vec{E} + \frac{1}{c}\vec{v}\times\vec{B}) \quad (2.11)$$

Calculating the cross product

$$\vec{v}\times\vec{B} = (v_y\cdot\partial A_y/\partial x, v_x\cdot\partial A_y/\partial x, 0) \quad (2.12)$$

we can now separate 2.11 into two components

$$dp_x/dt = -v_y \cdot \partial A_y/\partial x \tag{2.13}$$

and

$$\begin{aligned} dp_\perp/dt = \partial A/\partial t + v_x \cdot \partial A/\partial x = \\ \partial A/\partial t + dx/dt \cdot \partial A/\partial x = \\ dA/dt \end{aligned} \tag{2.14}$$

We see that $p_\perp - A = p_{\perp 0}$, as if no inertia was present, which already simplifies the motion of the particle.
The conservation of energy gives us

$$\begin{aligned} d(\gamma \cdot m \cdot c^2)/dt = -e \cdot (\vec{v} \cdot \vec{E}) \Leftrightarrow \\ d\gamma/dt = -\vec{v} \cdot \vec{E} \end{aligned} \tag{2.15}$$

If we subtract (2.11) from () we get

$$\begin{aligned} \frac{d}{dt}(p_x - \gamma) = \\ dp_x/dt - d\gamma/dt = \\ -v_y \cdot \partial A_y/\partial x - v_y \cdot \partial A_y/\partial t = \\ -v_y \cdot (\partial/\partial x - \partial/\partial t) A_y = 0 \end{aligned}$$

Therefore

$$p_x - \gamma = -\alpha = cte \tag{2.16}$$

Now, if we choose $p_x = p_{\perp 0} = 0$, then $\gamma_0 = 1$, which implies that $\alpha = 1$. The Lorentz factor relates to the momentum through

$$\gamma^2 = 1 + p^2 = 1 + p_x^2 + p_\perp^2 \tag{2.17}$$

Writing 2.11 in terms of γ, substituting in 2.11 and rearranging terms, we get

$$2 \cdot \omega_0 \cdot p_x - p_\perp^2 = 0 \tag{2.18}$$

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