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# Appendices

# Appendix A

#### Fermi Acceleration

#### A.1 Second Order Fermi Acceleration

The Fermi mechanism <sup>1</sup> was first proposed by Fermi in 1949 as a stochastic means by which particles colliding with clouds in the interstellar medium could be accelerated to high energies. We will consider two versions of the mechanism. In this section, we consider Fermi's original version of the theory, the problems it encounters and how it can be reincarnated in a modern guise. The analysis contains some features which are important for particle acceleration in general.

In Fermi's original picture, charged particles are reflected from 'magnetic mirrors' associated with irregularities in the Galactic magnetic field. The mirrors are assumed to move randomly with typical velocity V, and Fermi showed that the particles gain energy statistically in these in these reflections. If the particles only remain within the acceleration region for some characteristic time  $\tau_{esc}$ , a power-law distribution of the particle energies is found.

<sup>&</sup>lt;sup>1</sup>Modified from Longair (1994)

Let us repeat Fermi's original calculation, in which the collision between the particle and a mirror, or massive cloud, takes place such that the angle between the initial direction of the particle and the normal to the surface of the mirror is  $\theta$ , as illustrated in Figure (A.1(a)). Let us work out the change of energy of the particle in a single collision. It is important to carry out a proper relativistic analysis.

We suppose the cloud is infinitely massive so that its velocity is unchanged in the collision. The center of momentum frame is therefore that of the cloud moving at the velocity V. The energy of the particle in this frame is

$$E' = \gamma_V (E + V p \cos \theta) \tag{A.1}$$

where

$$\gamma_V = \left(1 - \frac{V^2}{c^2}\right)^{-1/2}$$
(A.2)

The x component of the relativistic three-momentum in the center of momentum frame is

$$p'_{x} = p' \cos \theta' = \gamma_{V} \left( p \cos \theta + \frac{VE}{c^{2}} \right)$$
 (A.3)

In the collision, the particle's energy is conserved,  $E'_{before} = E'_{after}$ , and its momentum in the x direction is reversed,  $p'_x \to -p'_x$ . Therefore, transforming back to the observer's frame, we find

$$E'' = \gamma_V (E' + V p'_x) \tag{A.4}$$

Substituting equations (A.1) and (A.3) in to equation (A.4) and recalling that  $p_x/E = v \cos \theta/c^2$ , we can find the change in energy of the particle

$$E'' = \gamma_V^2 E \left[ 1 + \frac{2Vv\cos\theta}{c^2} + \left(\frac{V}{c}\right)^2 \right]$$
(A.5)

Expanding to second order in V/c, we find

$$E'' - E = \Delta E = \frac{2Vv\cos\theta}{c^2} + 2\left(\frac{V}{c}\right)^2 \tag{A.6}$$



Figure A.1: Illustrating the collision between a particle of mass m and a cloud of mass M. (a) A head-on collision; (b) a following collision. The probabilities of head-on and following collisions are proportional to the relative velocities of approach of the particle and the cloud, namely,  $v + V \cos \theta$  for (a) and  $v - V \cos \theta$ for (b). Since  $v \approx c$ , the probabilities are proportional to  $1 + (V/c) \cos \theta$ , where  $0 < \theta < \pi$ 

We now have to average over the angle  $\theta$ . Because of scattering by hydromagnetic waves or irregularities in the magnetic field, it is likely that the particle is randomly scattered in pitch angle between encounters with the clouds, and we can therefore work out the mean increase in energy by averaging over the angle  $\theta$  in the expression (A.6). A crucial point is that there is a slightly greater probability of head-on encounters as opposed to the following collisions (Figure A.1). It will be observed that the probability of encounters taking place at an angle of incidence  $\theta$  is given by exactly the same reasoning which led to rate of arrival of photons at an angle  $\theta$  in the our analysis of inverse Compton scattering. The only difference is that the particles more at a velocity v rather than c. For simplicity, let us consider the case of a relativistic particle with  $v \approx c$ , in which case the probability of collision at angle  $\theta$  is proportional to  $\gamma_V[1 + (V/c)\cos\theta]$ . Recalling that the probability of the pitch angle lying in the angular range  $\theta$  to  $\theta + d\theta$  is proportional to  $\sin \theta \, d\theta$ , we find on averaging over all angles in the range 0 to  $\pi$ that the first term in expression (A.6) in the limit  $v \to c$  becomes

$$\left\langle \frac{2V\cos\theta}{c} \right\rangle = \left(\frac{2V}{c}\right) \frac{\int_{-1}^{1} x[1 + (V/c)x] \, dx}{\int_{-1}^{1} [1 + (V/c)x] \, dx} = \frac{2}{3} \left(\frac{V}{c}\right)^2 \tag{A.7}$$

where  $x = \cos \theta$ . Thus, in the relativistic limit, the average energy gain per collision is

$$\left\langle \frac{\Delta E}{E} \right\rangle = \frac{8}{3} \left( \frac{V}{c} \right)^2$$
 (A.8)

This illustrates the famous result derived by Fermi that the average increase in energy is only second order in V/c. It is also immediately apparent that this result leads to an exponential increase in the energy of the particle since the same fractional increase occurs per collision. Before looking at this part of the calculation a little more deeply, let us complete the essence of Fermi's original argument. If the mean free path between clouds along a field line is L, the time between collisions is  $L/(c \cos \phi)$ , where  $\phi$  is the pitch angle of the particle with respect to the magnetic field direction. We need to average  $\cos \phi$  over the pitch angle  $\phi$  to find the average time between collisions, which is just 2L/c. Therefore, we fine a typical rate of energy increase

$$\frac{dE}{dt} = \frac{4}{3} \left( \frac{V^2}{cL} \right) E = \alpha E \tag{A.9}$$

It is assumed that the particle remains in the accelerating region for a characteristic time  $\tau_{esc}$ . We now write down the diffusion-loss equation (19.13) and find the solution for N(E) in equilibrium, that is,

$$\frac{dN}{dt} = D\nabla^2 N + \frac{\partial}{\partial E} [b(E)N(E)] - \frac{N}{\tau_{esc}} + Q(E)$$
(A.10)

We are interested in the steady-state solution and, hence, dN/dt = 0. We are not interested in diffusion and, hence,  $D\nabla^2 N = 0$ , and we assume there are no sources, Q(E) = 0. The energy loss term is b(E) = -dE/dt, which in our case is  $-\alpha E$ . Therefore, equation (A.10) reduces to

$$-\frac{d}{dE}[\alpha EN(E)] - \frac{N(E)}{\tau_{esc}} = 0$$
(A.11)

Differentiating and rearranging this equation, we find

$$\frac{dN(E)}{dE} = -\left(1 + \frac{1}{\alpha \tau_{esc}}\right) \frac{N(E)}{E}$$
(A.12)

Therefore

$$N(E) = \text{constant} \times E^{-x} \tag{A.13}$$

where  $x = 1 + (\alpha \tau_{esc})^{-1}$ . It can be seen that we have succeeded in deriving a power-law energy spectrum.

#### A.2 Particle acceleration in strong shocks: The

#### first order Fermi acceleration

We can rewrite the essence of the Fermi mechanism in a rather simpler fashion if we let  $E = \beta E_0$  be the average energy of the particle after one collision and P be the probability that the particle remains within the accelerating region after one collision. Then, after k collisions, there are  $N = N_0 P^k$  particles with energies  $E = E_0 \beta^k$ . If we eliminate k between these quantities,

$$\frac{\ln(N/N_0)}{\ln(E/E_0)} = \frac{\ln P}{\ln \beta} \tag{A.14}$$

and hence

$$\frac{(N)}{N_0} = \left(\frac{E}{E_0}\right)^{\ln P / \ln \beta} \tag{A.15}$$

In fact, this value of N is  $N(\geq E)$  since this number reach energy E and some fraction of them go on to higher energies. Therefore

$$N(E)dE = \text{constant} \times E^{-1 + (\ln P / \ln \beta)} dE$$
(A.16)

It is clear in this formulation that we have again recovered a power law. To make the equivalence between the first and second versions of Fermi acceleration complete, we see that, from Equation (A.13) and the definition of  $\beta$ ,  $\beta = 1 + (\alpha/M)$ , where  $\alpha/M$  is the increment in energy per collision and P is related to  $\tau$ .

In the version of the of the Fermi mechanism described in previous section,  $\alpha$  is proportional to  $(V/c)^2$ , because of the decelerating effect of the following collisions.

The original version of Fermi's theory is therefore known as second order Fermi acceleration and clearly is a very slow process. We would do much better if there were only head-on collisions. In this case, the energy increase is  $\Delta E/E \propto$  2V/c, that is, first order in V/c, and, appropriately, this is called *first order Fermi* acceleration.

A very attractive version of first order Fermi acceleration in the presence of strong shock waves was discover independently by a number of workers in the late 1970s. The papers by Axford, Leer and Skadron (1977), Krymsky (1977), Bell (1978) and Blandford and Ostriker (1978) stimulated an enormous amount of interest in this process for the many environments in which high energy particles are found in astrophysics. There are two different ways of tackling the problem, one starting from the diffusion equation for the evolution of the momentum distribution of high energy particles in the vicinity of a strong shock (for example, Blandford and Ostriker (1978)) and the other, a more physical approach, in which the behavior of individual particles is followed (for example, Bell (1978)). I will adopt Bell's version of the theory, which makes the essential physics clear and indicates why this version of first order Fermi acceleration results remarkably naturally in a power-law energy spectrum of high energy particles.

To illustrate the basic physics of the acceleration process, let us consider the case of a strong shock, for example, that caused by a supernova explosion, propagating through the interstellar medium. A flux of high energy particles is assumed to be present both in front of and behind the shock front. The particles are considered to be of very high energy, and so the velocity of the shock is very much less than the velocities of the high energy particles. The key point about the acceleration mechanism is that the high energy particles hardly notice the shock at all, since its thickness will normally be very much smaller than the gyroradius of a high energy particle. Because of turbulence behind the shock front and irregularities ahead of it, when the particle pass through the shock in either direction, they are scattered so that their velocity distribution rapidly becomes isotropic on either side of the shock front. The key point is that the distributions are isotropic with respect to the frames of reference in which the fluid is at rest on either side of the shock.

Let us consider the case of a strong shock. This is the case, for example, for the material ejected in supernova explosions, where the velocities can be up to about 10<sup>4</sup> km s<sup>-1</sup>, compared with the sound and Alfven speeds of the interstellar medium, which are at most about 10 km s<sup>-1</sup>. In the case of a strong shock, the shock wave travels at a highly supersonic velocity  $U \gg c_s$ , where  $c_s$  is the sound speed in the ambient medium Figure (A.2(a)). It is often convenient to transform into the frame of reference in which the shock front is at rest, and then the upstream gas flows into the shock front at velocity  $v_1 = U$  and leaves the shock with a downstream velocity  $v_2$  (Figure A.2(b)). The equation of continuity requires mass to be conserved through the shock, and so

$$\rho_1 v_1 = \rho_2 v_2 \tag{A.17}$$

In the case of a strong shock,  $\rho_2/\rho_1 = (\gamma + 1)/(\gamma - 1)$ , where  $\gamma$  is the ratio of specific heats of the gas. Taking  $\gamma = 5/3$  for a monatomic of fully ionized gas, we find  $\rho_2/\rho_1 = 4$ , and so  $v_2 = \frac{1}{4}v_1$ .

Now let us consider the high energy particles ahead of the shock. Scattering ensures that the particle distribution is isotropic in the frame of reference in which the gas is at rest. It is instructive to draw diagrams illustrating the dynamical situation so far as typical high energy particles upstream and downstream of the shock are concerned. Let us consider the upstream particles first. The shock advances through the medium at velocity U, but the gas behind the shock travels at a velocity (3/4)U relative to the upstream gas (Figure A.2(c)). When a high energy particle crosses the shock front, it obtains a small increase in energy of the order  $\Delta E/E \sim U/c$ , as we will show below. The particles are then scattered by the turbulence behind the shock front so that their velocity distributions become isotropic with respect to that flow.

Now let us consider the opposite process of the particle diffusing from behind the shock to the upstream region in front of the shock (Figure A.2(d)). Now the velocity distribution of the particles is isotropic behind the shock. and, when they cross the shock front, they encounter gas moving towards the shock front, again with the same velocity, (3/4)U. In other words. the particle undergoes exactly the same process of receiving a small increase in energy  $\Delta E$  crossing the shock from downstream to upstream as it did in traveling from upstream to downstream. This is the clever aspect of this acceleration mechanism. Every time the particle crosses the shock front it receives an increase of energy - there are never crossing in which the particles lose energy - and the increment in energy is the same going in both directions. Thus, unlike the standard Fermi mechanism in which there are both head-on and following collisions, in the case of the shock front, the collisions are always head on and energy is transferred to the particles. The beauty of the mechanism is the complete symmetry between the passage of the particles from upstream to downstream and from downstream to upstream through the shock wave.

Let us now be somewhat more quantitative about the actual process of acceleration. By simple arguments, due originally to Bell (1978), we can work out both  $\beta$  and P for this cycle. First, we evaluate the average increase in energy of the particle on crossing from the upstream to the downstream sides of the shock. The gas on the downstream side approaches the particle at a velocity  $V = \frac{3}{4}U$  and so, performing a Lorentz transformation, the particle's energy when it passes into the downstream region is

$$E' = \gamma v (E + p_x V) \tag{A.18}$$

where we take the x coordinate to be perpendicular to the shock. We assume that the shock is non-relativistic,  $V \ll c$ ,  $\gamma v = 1$  but that the particles are relativistic, so that we can write E = pc,  $p_x = (E/c) \cos \theta$ . Therefore,

$$\Delta E = pV\cos\theta; \qquad \frac{\Delta E}{E} = \frac{V}{c}\cos\theta$$
 (A.19)

We now seek the probability that the particles which cross the shock arrive at an angle  $\theta$  per unit time. This is a standard piece of kinetic theory. The number of particles within the angles  $\theta$  to  $\theta + d\theta$  is proportional to  $\sin \theta d\theta$ , but the rate at which they approach the shock front is proportional to the x component of their velocities,  $c \cos \theta$ . Therefore the probability of the particle crossing the shock is proportional to  $\sin \theta \cos \theta d\theta$ . Normalizing so that the integral of the probability distribution over all the particles approaching the shock is equal to unity, that is, those with  $\theta$  in the range 0 to  $\pi/2$ , we find

$$p(\theta) = 2\sin\theta\cos\theta d\theta \tag{A.20}$$

Therefore, the average gain in energy on crossing the shock is

$$\left\langle \frac{\Delta E}{E} \right\rangle = \frac{V}{c} \int_0^{\pi/2} 2\cos^2\theta \sin\theta d\theta = \frac{2}{3} \frac{V}{c}$$
 (A.21)

The particle's velocity vector is randomized without any energy loss by scattering in the downstream region and it then recross the shock, as illustrated in Figure (A.2(d)), when it gains another fractional increase in energy  $\frac{2}{3}(V/c)$  so that, in making one round trip across the shock and back again, the fractional energy increase is, on average,

$$\left\langle \frac{\Delta E}{E} \right\rangle = \frac{4}{3} \frac{V}{c} \tag{A.22}$$

Consequently,

$$\beta = \frac{E}{E_0} = 1 + \frac{4V}{3c} \tag{A.23}$$

in one round trip.

To work out the escape probability P, we use a clever argument due to Bell (1978). According to classical kinetic theory, the number of particles crossing the shock is  $\frac{1}{4}Nc$ , where N is the number density of particles. This is the average number of particles crossing the shock in either direction, since, as noted above, the particles scarcely notice the shock. Downstream, however, the particles are swept away, or "advected", from the shock because the particles are isotropic in that frame. Referring to Figure (A.2(b)), it can be seen that the particles are removed from the region of the shock at a rate  $NV = \frac{1}{4}NU$ . Thus, the fraction of the particles lost per unit time is  $\frac{1}{4}NU/\frac{1}{4}Nc = U/c$ . Since we assume that the shock is non-relativitistic, it can be seen that only a very small fraction of the particles is lost per cycle. Thus, P = 1 - (U/c). This solves the problem since we need  $\ln \beta$  and  $\ln P$  to insert into expression (A.16). Therefore, since  $\ln P = \ln \left(1 - \frac{U}{c}\right) = -\frac{U}{c}$  and  $\ln \beta = \ln \left(1 + \frac{4V}{3c}\right) = \frac{4V}{3c} = \frac{U}{c}$  we find

$$\frac{\ln P}{\ln \beta} = -1 \tag{A.24}$$

and, hence, the differential energy spectrum of the high energy particles is

$$N(E)\mathrm{d}E \propto E^{-2}\mathrm{d}E \tag{A.25}$$

This is the result we have been seeking. It may be objected that we have obtained a value of 2 rather than 2.5 for the exponent of the differential energy spectrum, and that problem cannot be neglected. However, the reason that this mechanism has excited so much interest is that, for the first time, there are excellent physical reasons why power-law energy spectra with a unique spectral index should occur in diverse astrophysical environments. In this simplest version of the theory, the only requirements are the presence of strong shock waves and that the velocity vectors of the high energy particles be randomized on either side of the shock. It is entirely plausible that there are strong shocks in most sources of high energy particles, supernova remnants, active galactic nuclei and the diffuse components of extended radio sources.



Figure A.2: The dynamics of high energy particles in the vicinity of a strong shock wave. (a) A strong shock wave propagating at a supersonic velocity, U, through stationary interstellar gas with density  $\rho_1$ , pressure  $p_1$  and temperature  $T_1$ . The density, pressure and temperature behind the shock are  $p_2$ ,  $\rho_2$  and  $T_2$ , respectively. (b) The flow of interstellar gas in the vicinity of the shock front in the reference frame in which the shock front is at rest. In this frame of reference, the ratio of the upstream to the downstream velocity is  $v_1/v_2 = (\gamma + 1)/(\gamma - 1)$ . For a fully ionized plasma,  $\gamma = 5/3$  and the ratio of these velocities is  $v_1/v_2 = 4$ as shown. (c) The flow of gas as observed in the frame of reference in which the upstream gas is stationary and the velocity distribution of the high energy particles is isotropic. (d) The flow of gas as observed in the frame of reference in which the downstream gas is stationary and the velocity distribution of high energy particles is isotropic.

### Appendix B

### **Finite Difference Method**

Difference schemes can be developed using Taylor series<sup>1</sup>. This approach is especially useful for deriving finite difference approximations of exact derivatives (both total derivatives and partial derivatives) that appear in differential equations.



Figure B.1: Discretized x space.

Difference formulas for functions of a single variable, for example f(x), can be developed from the Taylor series for a function of a single variable:

$$f(x) = f_0 + f'|_0 \Delta x + \frac{1}{2} f''|_0 \Delta x^2 + \dots + \frac{1}{n!} f^{(n)}|_0 \Delta x^n + \dots$$
(B.1)

where  $f_0 = f(x_0), f'(x_0)$ , and so on. The continuous spatial domain D(x) must be discretized into an equally spaced grid of discrete points, as illustrated in

<sup>&</sup>lt;sup>1</sup>This part was copied from Hoffman (1992).

Figure (B.1). For the discrete grid,

$$f(x_i) = f_i \tag{B.2}$$

where the subscript *i* denotes a particular spatial location. The Taylor series for f(x) at grid points surrounding point *i* can be combined to obtain difference formulas for  $f'(x_i), f''(x_i), etc.$ 

Difference formulas for functions of several variables, for example f(x, t), can be developed from the Taylor series for a function of several variables. For the two-variable function f(x, t), the Taylor series is give by

$$f(x,t) = f_0 + (f_x|_0 \Delta x + f_t|_0 \Delta t) + \frac{1}{2} (f_{xx}|_0 \Delta x^2 + 2f_{xt}|_0 \Delta x \Delta t + f_{tt}|_0 \Delta t^2) + \dots + \frac{1}{n!} (f_{(n)x}|_0 \Delta x^n + \dots + f_{(n)t}|_0 \Delta t^n) + \dots$$
(B.3)

where  $f_0 = f(x_0, t_0)$ ,  $f_{(n)x}$  denotes  $\partial^n f / \partial x^n$ , and so on. The continuous domain D(x, t) must be discretized into an orthogonal equally spaced grid of discrete points (i, n) (*i* and *n* are the spatial and time indices) can be combined to obtain difference formulas for  $f_x$ ,  $f_t$ , etc.

For partial derivatives of f(x,t) with respect to  $x, t = t_0$  =constant,  $\Delta t = 0$ , and Equation (B.3) becomes

$$f(x,t_0) = f_0 + f_x|_0 \Delta x + \frac{1}{2}f_{xx}|_0 \Delta x^2 + \dots + \frac{1}{n!}f_{(n)x}|_0 \Delta x^n + \dots$$
(B.4)

Equation (B.4) is identical in form to Equation (B.1), where  $f'|_0$  corresponds to  $f_x|_0$ , etc. The partial derivative  $f_x|_0$  of the function f(x, t) can be obtained from Equation (B.4) in exactly the same manner as the total derivative  $f'|_0$  of the function f(x) is obtained from Equation (B.1). Since Equation (B.1) and B.4 are identical in form, the difference formulas for  $f'|_0$  and  $f_x|_0$  are identical if the same

discrete grid points are used to develop the difference formulas. Consequently, difference formulas for partial derivatives of a function of several variables can be derived from the Taylor series for a function of a single variable. To emphasize this concept, the following common notation for derivatives will be used in the development of difference formulas for total derivatives and partial derivatives:

$$\frac{d}{dx}(f(x)) = f_x \tag{B.5}$$

$$\frac{\partial}{\partial x}(f(x,t)) = f_x \tag{B.6}$$

In a similar manner, partial derivatives of f(x, t) with respect to t can be obtained from the expression

$$f(x_0, t) = f_0 + f_t|_0 \Delta t + \frac{1}{2} f_{tt}|_0 \Delta t^2 + \dots + \frac{1}{n!} f_{(n)t}|_0 \Delta t^n + \dots$$
(B.7)

Partial derivatives of f(x, t) with respect to t are identical in form to total derivatives of f(t) with respect to t. This approach does not work for mixed partial derivatives, such as  $f_{xt}$ . Difference formulas for mixed partial derivatives must ba determined directly from the Taylor series for several variables. The Taylor series for the function f(x), Equation (B.1), can be written as

$$f(x) = f_0 + f_x|_0 \Delta x + \frac{1}{2} f_{xx}|_0 \Delta x^2 + \dots + \frac{1}{n!} f_{(n)x}|_0 \Delta x^n + \dots$$
(B.8)

$$f(x) = f_0 + f_x|_0 \Delta x + \frac{1}{2} f_{xx}|_0 \Delta x^2 + \dots + \frac{1}{n!} f_{(n)x}|_0 \Delta x^n + R_{n+1}$$
(B.9)

The Taylor formula with remainder is where the remainder term  $R_{n+1}$  is given by

$$R_{n+1} = \frac{1}{(n+1)!} f_{(n+1)x}(\xi) \Delta x^{n+1}$$
(B.10)

where  $x_0 \leq \xi \leq x_0 + \Delta x$ .



Figure B.2: Discretized xt space.

The infinite Taylor series Equation (B.8) and the Taylor formula with remainder Equation (B.9) are equivalent. The error incurred by truncating the infinite Taylor series after the *n*th derivative is exactly the remainder term of the *n*th-order Taylor formula. Truncating the Taylor series is equivalent to dropping the remainder term of the Taylor formula. Finite difference approximations of exact derivatives can be obtained by solving for the exact derivative from either the infinite Taylor series or the Taylor formula, and then either truncating the Taylor series or dropping the remainder term of the Taylor formula. These two procedures are identical. The terms that are truncated from the infinite Taylor series, which are identical to the remainder term of the Taylor formula, are called the *truncation error* of the finite difference approximation of the exact derivative. In most cases, our main concern is the order of the truncation error, which is the rate at which the truncation error approaches zero as  $\Delta x \rightarrow 0$ . The order of the truncation error, which is the order of the remainder term, is denoted by the notation  $O(\Delta x^n)$ . Consider the equally spaced discrete finite difference grid



Figure B.3: Discretized t space.

illustrated in Figure (B.2). Choose point *i* as the base point and write the Taylor series for  $f_{i+1}$  and  $f_{i-1}$ :

$$f_{i+1} = f_i + f_x|_i \Delta x + \frac{1}{2} f_{xx}|_i \Delta x^2 + \frac{1}{6} f_{xxx}|_i \Delta x^3 + \frac{1}{24} f_{xxxx}|_i \Delta x^4 + \dots$$
(B.11)

$$f_{i-1} = f_i - f_x|_i \Delta x + \frac{1}{2} f_{xx}|_i \Delta x^2 - \frac{1}{6} f_{xxx}|_i \Delta x^3 + \frac{1}{24} f_{xxxx}|_i \Delta x^4 - \dots$$
(B.12)

Subtracting  $f_{i-1}$  from  $f_{i+1}$  gives

$$f_{i+1} - f_{i-1} = 2f_x|_i \Delta x + \frac{1}{3}f_{xxx}|_i \Delta x^3 + \dots$$
(B.13)

Letting the  $f_{xxx}$  term be the remainder term and solving for  $f_x|_i$  yields

$$f_x|_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} - \frac{1}{6}f_{xxx}(\bar{\xi})\Delta x^2$$
(B.14)

where  $x_{i-1} \leq \bar{\xi} \leq x_{i+1}$ . Equation (B.14) is an exact expression for  $f_x|_i$ . If the remainder term is dropped, which is equivalent to truncating the infinite Taylor series, Equations (B.11) and (B.12), Equation (B.14) yields a finite difference approximation of  $f_x|_i$ . Adding  $f_{i+1}$  and  $f_{i-1}$  gives

$$f_{i+1} + f_{i-1} = 2f_i + f_{xx}|_i \Delta x^2 + \frac{1}{12}f_{xxx}|_i \Delta x^4 + \dots$$
(B.15)

Letting the  $f_{xxx}$  term be the remainder term and solving for  $f_{xx}|_i$  yields

$$f_{xx}|_{i} = \frac{f_{i+1} - 2f_{i} + f_{i-1}}{\Delta x^{2}} - \frac{1}{12}f_{xxxx}(\xi)\Delta x^{2}.$$
 (B.16)

Equations (B.14) and (B.16) are centered-difference formulas. They are inherently more accurate than one-sided difference formulas. Equations (B.14) and (B.16) are difference formulas for spatial derivatives. Difference formulas for *time* derivatives can be developed in a similar manner. The time dimension can be discretized into a discrete temporal grid, as illustrated in Figure (B.3), where the superscript n denotes a specific value of time. Thus,

$$f(t^n) = f^n \tag{B.17}$$

Choose point n as the base point, and write the Taylor series for  $f^{n+1}$  and  $f^{n-1}$ :

$$f^{n+1} = f^n + f_t |^n \Delta t + \frac{1}{2} f_{tt} |^n \Delta t^2 + \dots$$
 (B.18)

$$f^{n-1} = f^n - f_t |^n \Delta t + \frac{1}{2} f_{tt} |^n \Delta t^2 - \dots$$
 (B.19)

Letting the term  $f_{tt}$  be the remainder term and solving Equation (B.18) for yields

$$f_t|^n = \frac{f^{n+1} - f^n}{\Delta t} - \frac{1}{2} f_{tt}(\tau) \Delta t$$
 (B.20)

where  $t^n \leq \tau \leq t^{n+1}$ . Equation (B.20) is a first-order forward-difference formula for  $f_t|^n$ . Subtracting  $f^{n-1}$  from  $f^{n+1}$  gives

$$f^{n+1} - f^{n-1} = 2f_t |^n \Delta t + \frac{1}{3} f_{ttt} |^n \Delta t^3 + \dots$$
 (B.21)

Letting the  $f_{ttt}$  term be the remainder term and solving for  $f_t|^n$  yields

$$f_t|^n = \frac{f^{n+1} - f^{n-1}}{2\Delta t} - \frac{1}{6}f_{ttt}(\bar{\tau})\Delta t^2$$
(B.22)

where Equation (B.22) is a second-order centered-difference formula for  $f_t|^n$ . Centered-difference formulas are inherently more accurate than one-sided difference formulas, such as Equation (B.20).

Differnce formulas of any order, based on one-sided forward differces, one-sided backward differences, centered differences, nonsymmetrical differences, *etc.*, can be obtained by different combinations of the Taylor series for f(x) or f(t) at various grid points, Higher-order difference formulas require more grid points, as do formulas for higher-order derivatives.

#### Appendix C

### Source Code Program

field.c: This program provides some useful functions used in main program.

/\* August, 15, 2000 change argument term2 in several routine August 1, 2000 June 14, 2000 -- June 1st. 2000 Made correction following QA treatment added enratio() f\_cont.c -- December 3rd, 1999. New function, enratio() -> energy ratio, is called by elements(). Cosmetic changes. last modified --- Aug 15, 1999 na ja.. Probably this is the correct version of field.xxx for spherical shock problem. last modified --- Aug 14, 1999. f\_sphere.c --- Aug 10, 1999. Modify from f\_hybr.c and f\_cont.c New modification to suit spherical shock case. changed Omega...a solar self rotation cospsi(z,vsw): add new argument vsw diffcoeff(): call antideriv2(); antideriv2(): instead of antideriv(); mudot(...) add vsw: argument, declare focuslength, R\_up=Archimedian spiral constant on up and downstream region at any location z. f\_hybk.c (h) -- July 22, 1999.

New subroutines added for hybrid finite difference-orbit code (hybwind). Removed findpb(). Changed arguments to dzdt(). relvel() replaced by two functions, relvwf() and relvws(), giving the wind speed relative to the fixed or shock frame, respectively. Added thetam(vsw), thetap(vsw). f\_kink.c -- April 8, 1999. Added arguments to diffcoeff and findpb() for compatibility with latest varwind.c. f\_kink.c -- December 16, 1998. For use with new version of varwind. Replaced betaswc() with dzdt(). Added relvel(). f\_kink.c -- May 18, 1997. Trimmed out unnecessary #define variables and other cosmetic changes. f\_kink.c -- November 28, 1996. For use with varwind.c, and for a configuration with straight magnetic field lines with a kink corresponding to a shock. The solar wind is constant on either side. New routine: betaswc() -> solar wind speed / C parallel to z (parallel to B) WARNING: If deceleration is needed when using varwind.c, be sure to modify decelrate() according to the new def. used in decel(). Derived from f\_arc.c of July 12th, 1995. David Ruffolo Department of Physics Faculty of Science Chulalongkorn University Bangkok 10330, Thailand \*/ #include <math.h> С 0.1202 /\* in AU/min. \*/ #define (4.0\*atan(1.0))#define PI ZOFFSET #define 15.7951 /\* at a shock location \*/ /\* fluid speed / C along B downstream 0.00533333 #define BETAD z < Zshock) - MUST BE CONSISTENT w/ stream.c 1600 km/s \*/ 0.0013333 /\* fluid speed / C along B upstream #define BETAU (z > Zshock) - MUST BE CONSISTENT w/ stream.c should have BETASWU > BETASWD km/s \*/ 400 /\* 86.16 : atan(14.92820 #define THETAM 1.50377 shock-field angle at z<zsh (radians) \*/</pre> 1.30899 /\* 75.0 : atan(3.73205) #define THETAP shock-field angle at z>zsh (radians) \*/ 2.519479e-6 /\* the self solar rotation rate #define Omega

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```
where synoptic rot. rate =2Pi/26.75(day)=2.718581e-6 rad/sec
          and sideral rot. rate = 2Pi/26.75-2Pi/365.25(day)=2.519479e-6 rad/sec
                                    */
/* dzz
      THIS ROUTINE CALCULATES AN EFFECTIVE SPATIAL DIFFUSION
      COEFFICIENT, EXPRESSING THE STRENGTH OF THE PITCH
                         THIS USES THE LIMIT OF diffcoeff
      ANGLE SCATTERING.
      IN THE ABSENCE OF FOCUSING. THIS COEFFICIENT IS
      DIMENSIONLESS - IT SHOULD BE MULTIPLIED BY v*v/ampl.
*/
double
         dzz(mustep,q)
double
         mustep, q;
{
   double
            a1, a2, mu, out;
   double
            antideriv2();
   for (out=0.0,mu= -1.0+mustep;mu<1.0;mu+=mustep)</pre>
    out += 0.25 * (1.0-mu*mu)
     * ((a1=antideriv2(mu+mustep/2.0,q))
          - (a2=antideriv2(mu-mustep/2.0,q)));
   return(out);
}
/* diffcoeff
      THIS ROUTINE CALCULATES A MODIFIED SCATTERING COEFFICIENT.
      THE MODIFICATION SHOULD PROVIDE MORE ACCURATE f'S NEAR THE
      SINGULARITY AT mu = 0.
      NOTE: THIS IS NOT GOOD FOR q = 2.
*/
double
         diffcoeff(mu,mustep,aoverv,q,r,v,vsw)
double
         mu, mustep, aoverv, q, r, v, vsw;
Ł
   double
            a1, a2, out, arg, focuslength;
   double
            antideriv2();
            radius(), arclength(), z, f_length();
   double
   r = radius(z);
   z =arclength(r);
   focuslength = f_length(z,vsw);
   a1 = antideriv2(mu+mustep/2.0, q);
   a2 = antideriv2(mu-mustep/2.0, q);
   arg = (1.0/(2.0*aoverv*focuslength)) * (a1-a2);
   out = (1.0/(2.0*focuslength)) * (1.0-mu*mu) * (mustep/2.0) / tanh(arg);
   return(out);
}
/* antideriv2
```

This routine contains the antiderivative of the inverse of

```
(the diffusion coefficient divided by ampl*(1-mu*mu)).
      Note: this formula is not appropriate for q = 2.0 or 3.0.
*/
         antideriv2(mu,q)
double
double
         mu, q;
{
   void
            nrerror();
   if (q == 2.0) nrerror("antideriv: q = 2.0");
   return(mu*pow(fabs(mu),1.0-q)/(2.0-q));
}
/* mudot
      THIS ROUTINE CALCULATES THE RATE OF INCREASE OF mu DUE TO
      ADIABATIC FOCUSING.
      For the straight magnetic fields considered here,
*/
double
         mudot(v,mu,r,vsw)
double
         v, mu, r, vsw;
                               /* cospsi(z,vsw) */
   double cospsi();
   double focuslength;
                              /*
                                  1/L(z) = -1/B * dB/dz
                                                              */
   double out;
                     /* constant parameter for Archimedian spiral in up and
   double R_ud;
                        downstream region;
                     */
   double relvwf();
   double radius(), z, f_length(), arclength();
   z =arclength(r);
   focuslength = f_length(z,vsw);
   out= 0.5*v*(1.0-(mu*v*relvwf(z,vsw)*cospsi(z,vsw))/(C*C))/focuslength;
   out += (mu*relvwf(z,vsw))/r * (1.0-1.5*(1.0-cospsi(z,vsw)*cospsi(z,vsw)));
   out *= (1.0 - mu + mu)/v;
   return(out);
7
/* arclength
      FINDS THE PATHLENGTH ALONG AN IDEAL PARKER FIELD FROM THE SUN
      TO THE GIVEN RADIUS.
      For this configuration, we do not consider the radius,
      so we set z = r.
*/
double
         arclength(r)
double
         r;
{
   return(r - ZOFFSET);
}
/* radius
```

```
FOR A GIVEN PATHLENGTH ALONG AN IDEAL PARKER FIELD FROM THE SUN,
      FIND THE RADIUS.
      For this configuration, we do not consider the radius,
      so we set z = r.
*/
double
         radius(z)
double
         z;
Ł
   return(z + ZOFFSET);
}
/* cospsi
      FOR A GIVEN PATHLENGTH ALONG AN IDEAL PARKER FIELD FROM THE SUN,
      FIND THE COSINE OF THE FIELD'S ANGLE (ANGLE=0 IF RADIALLY OUTWARD).
*/
double
         cospsi(z,vsw)
double
         z, vsw;
{
    double r_updown(), R_ud, out;
    double radius(), r;
    r = radius(z);
    R_ud = r_updown(z,vsw);
    out=(R_ud / sqrt(R_ud*R_ud + r*r));
    return(out);
}
/* dsecdz
      d(sec(psi))/dz is zero for this configuration.
*/
double
         dsecdz(z)
double
         z;
ſ
   return(0.0);
}
/* zenith
      FOR A GIVEN PATHLENGTH ALONG AN IDEAL PARKER FIELD FROM THE SUN,
      FIND THE ZENITH ANGLE RELATIVE TO THE FLARE SITE (IN RADIANS).
      For this configuration, we do not consider the radius,
      so we set zenith = 0.
*/
double
         zenith(z)
double
         z;
ł
   return(0.0);
}
/* dzdt
       The Fokker-Planck coefficient, Delta z / Delta t.
*/
double
         dzdt(bet,mu,z,vsw)
```

```
bet, mu, z, vsw;
double
{
            relvwf(),cospsi();
   double
   double
            v, out;
    v= bet*C;
    out= mu*v*cospsi(z,vsw)+relvwf(z,vsw)-
           (mu*mu*v*v*relvwf(z,vsw)*cospsi(z,vsw)*cospsi(z,vsw))/(C*C);
    return(out);
}
/* relvwf is the velocity of the wind RELATIVE TO THE FIXED FRAME */
         relvwf(z,vsw)
double
double
         z, vsw;
£
   double
            radius(), out;
   if (z < ZOFFSET) {
      out = -BETAD*C;
   } else {
      out = -BETAU*C;
   7
   return(out);
}
/* relvws is the velocity of the wind RELATIVE TO THE SHOCK */
/* no need to use r right?
double
       relvws(z,vsw)
double
       z, vsw;
{
   double
           out;
   if (z < ZOFFSET) {
      out = -BETAD * C;
   } else {
      out = -BETAU*C;
   3
   return(out);
}
*/
        relvws(z,vsw)
double
double
       z, vsw;
Ł
   double
            out;
   if (z < ZOFFSET) {
      out = -BETAD * C;
   } else {
      out = -BETAU*C;
   }
   return(out);
7
/* thetam
      Return the angle between the magnetic field and the shock normal
      for z just < zsh (in radians).
```

```
*/
double
         thetam(vsw)
double
         VSW;
ł
   return(THETAM);
}
/* thetap
      Return the angle between the magnetic field and the shock normal
      for z just > zsh (in radians).
*/
double
         thetap(vsw)
double
         vsw;
{
   return(THETAP);
}
/* decelrate
      For this configuration, there is no deceleration away from the shock.
      as previous motion we set
      decelrate(xxx) = -p<delta p/delta t>
*/
          decelrate(z,mu,vsw)
double
double
         z, mu, vsw;
{
   double cospsi(), radius(), r;
   r=radius(z);
   return(-relvwf(z,vsw)*((0.5/r)*(1.0-(3.0*mu*mu))*
           (1.0-cospsi(z,vsw)*cospsi(z,vsw))-((1.0-mu*mu)/r)));
}
/* enratio - calculates the ratio of the particle energy in the local
    fluid frame to the energy in the fixed frame - used in the diffusion term.
*/
double
          enratio(mu,z,v,vsw)
double
         mu, z, v, vsw;
{
             relvwf();
   double
   return(1 - mu*v*relvwf(z,vsw)/(C*C));
}
/*
     This routine calculates focusing length
*/
         f_length(z,vsw)
double
double z, vsw;
{
   double r_updown(), R_ud, out;
   double r, radius();
   r = radius(z);
   R_ud = r_updown(z,vsw);
   out= (r * (R_ud*R_ud + r*r) * sqrt(R_ud*R_ud + r*r)) /
```

(R\_ud \* (2\*R\_ud\*R\_ud+r\*r));

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# Appendix D

#### Shock waves

A quantitative analysis <sup>1</sup> will be presented only for ordinary gas dynamic shocks for which  $\vec{B} = 0$ . This analysis will show that a gas goes from being supersonic upstream of the shock to subsonic downstream of the shock. We now have the following conservation relations:

$$[\rho u] = 0 \tag{D.1}$$

$$\left[\rho u^2 + p\right] = 0 \tag{D.2}$$

$$\left[\left(\frac{1}{2}\rho u^2 + \frac{\gamma}{\gamma - 1}p\right)u\right] = 0 \tag{D.3}$$

Equation (D.1) is equivalent to

$$\rho_1 u_1 = \rho_2 u_2 \quad \text{or} \quad \frac{u_2}{u_1} = \frac{\rho_1}{\rho_2} = 1/Z_s,$$
(D.4)

where we have introduced the ratio  $Z_s \equiv \rho_2/\rho_1$  which is the density "jump" or "shock jump" across the shock. The velocity jump is inversely proportional to  $Z_s$  Equations (D.2) and (D.3) can also be written in terms of the upstream and

<sup>&</sup>lt;sup>1</sup>Copied from Cravens 1997

downstream values of the fluid variables (see Figure D.1):

$$\rho_1 u_1^2 + p_1 = \rho_1 u_2^2 \tag{D.5}$$

$$\left(\frac{1}{2}\rho_1 u_1^2 + \frac{\gamma}{\gamma - 1}p_1\right) u_1 = \left(\frac{1}{2}\rho_2 u_2^2 + \frac{\gamma}{\gamma - 1}p_2\right) u_2.$$
(D.6)

Let us suppose that all the upstream variables,  $\rho$ ,  $u_1$ , and  $p_1$  are known. Then Equations (D.4)-(D.6) constitute three equations that can be used to solve for the three unknowns,  $\rho_2$ ,  $u_2$ , and  $\rho_2$ . In fact,  $\rho_2$ ,  $u_2$ , and  $p_2$  can all be found in terms of the upstream sonic Mach number  $M_1$ . We have

$$M_1^2 = \frac{\rho_1 u_1^2}{\gamma p_1}$$
 and  $M_2^2 = \frac{\rho_2 u_2^2}{\gamma p_2}$ . (D.7)

where  $\gamma =$  specific heat, Equations (D.4)-(D.6) can be solved to obtain

$$\frac{u_2}{u_1} = \frac{\gamma - 1}{\gamma + 1} + \frac{2}{(\gamma + 1)M_1^2}.$$
 (D.8)

Hence, from Equation (D.4) the shock jump  $Z_s$  is

$$Z_s = \frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} = \frac{\gamma + 1}{\gamma - 1 + \frac{2}{M_1^2}}.$$
 (D.9)

We can also use these results to find the pressure jump, which is

$$\frac{p_2}{p_1} = \frac{2\gamma M_1^2 - (\gamma - 1)}{\gamma + 1}.$$
 (D.10)

Equations (D.8)-(D.10) are called the Rankine-Hugoniot relations.

For  $M_1 = 1$ , we have  $u_2/u_1 = \rho_2/\rho_1 = p_2/p_1 = 1$ ; there is no shock and the flow stays sonic  $(u = C_s)$ . We cannot have  $M_1^2 < 1$ . But for  $M_1 > 1$  we have  $Z_s > 1$ , indication that the density increases and the flow speed decrease across the shock (see Figure D.1). Naturally, the mass flux must remain constant across a steady-state shock in order to prevent mass build-up (or loss) at the discontinuity surface. Because the flow decelerates at the shock there is compression. Compression and slowdown are associated with an increase in pressure



Figure D.1: Schematic of shock wave showing the jump in density and a drop in velocity.

(and temperature). The temperature jump across the shock can be derived from Equation (D.10) and a suitable equation of state. For ordinary air,  $p = \rho \tilde{R}T_n$ , but for a plasma  $p = p_e + p_i = \rho \frac{k_B}{m_i}(T_e + T_i)$ , where  $m_i$  using the ion-acoustic speed, which includes both  $T_e$  and  $T_i$ .

The hypersonic limits of the Rankine-Hugoniot relations can be found by taking the limit  $M_1^2 \to \infty$ :

$$\lim_{M_1^2 \to \infty} Z_s = \frac{\rho_1}{\rho_2} = \frac{u_1}{u_2} \to \frac{\gamma + 1}{\gamma - 1} (= 4 \text{ for } \gamma = 5/3).$$
(D.11)

The maximum shock jump for  $\gamma = 5/3$ , is 4, but the maximum pressure jump is infinite:

$$\lim_{M_1^2} \frac{p_2}{p_1} = \frac{2\gamma}{\gamma+1} M_1^2 \to \infty.$$
(D.12)

For supersonic flow upstream of the shock, the downstream flow must be subsonic, as we can see by rearranging the Rankine-Hugoniot relation to get

$$M_2^2 = \frac{(\gamma - 1)M_1^2 + 2}{2\gamma M_1^2 - (\gamma - 1)}.$$
 (D.13)

Clearly, this equation shows that the downstream gas flow is subsonic  $(M_2 < 1)$  for upstream gas flow that is supersonic  $(M_1 > 1)$ . The hypersonic limit of the downstream Mach number is  $(M_2^2 \rightarrow (\gamma - 1)/(2\gamma))$ , which is equal to 1/5 for an ideal monatomic gas with  $\gamma = 5/3$ .

Gas flow across a shock is thermodynamically irreversible; that is, the net change of entropy is positive and nonzero. The quantity  $p/\rho^{\gamma}$  is related to the entropy per unit mass (or *specific entropy*). Specific entropy is a constant for small perturbations such as typical sound waves. The flow is then said to be *isentropic*. However, the specific entropy increases across a shock:

$$\frac{p_2}{\rho_2^{\gamma}} > \frac{p_1}{\rho_1^{\gamma}} \tag{D.14}$$

Irreversible "dissipation" of bulk kinetic energy  $(\rho u^2)$  into thermal energy (p) takes place inside the shock discontinuity. This dissipation is related to collisions in an ordinary shock wave, but in space plasmas, the shocks are collisionless, and the nature of the dissipation mechanism becomes tricky. Nonetheless, shock do exist in space and thus dissipation must be present, albeit associated with microscopic plasma instabilities and waves (i.e., small-scale structure in the plasma and fields) rather than ordinary collisions.

We have just analyzed ordinary gas shocks, but what about MHD shocks in general? The conservation relations are much messier if we ratain the magnetic field terms. However, for *parallel shocks*  $(\vec{B} \parallel \vec{u})$  the field again drops out of the equations and we re-obtain the Rankine-Hugoniot relations for an ordinary shock. But, as just discussed, the dissipation mechanism for parallel, collisionless shocks in space plasma is problematic (and not very efficient). Parallel shocks observed in space are not really discontinuities but appear as quite thick layers that had considerable plasma turbulence associated with them, as required for the dissipation.

Dissipation for collisionless *perpendicular shocks*  $(\vec{B} \perp \vec{u})$  is more efficient than for parallel shocks and is associated with ion gyration. The shock thickness for this category of shock is roughly equal to an ion gyroradius. The MHD version of the Rankine-Hugoniot relations can be found from the appropriate conservation relations but will not be shown here. However, just as for ordinary shocks, the density increases and the velocity decreases across the shock. The change in the magnetic field can be written with  $B_n = 0$  (and  $u = u_n$ ,  $B = B_t$ )as:

$$u_1B_1 = u_2B_2$$
 or  $\frac{B_2}{B_1} = \frac{u_1}{u_2} = \frac{\rho_2}{\rho_1} = Z_s.$  (D.15)

The magnetic field jump is the same as the density jump. The general case is not simple but the hypersonic limit is the same as for ordinary shocks,  $Z_s =$   $(\gamma+1)/(\gamma-1)$ 

Oblique MHD shocks (in which the magnetic field is neither parallel to nor perpendicular to the flow) are even more complicated than perpendicular shocks. There are even two types for oblique shocks, one associated with slow-mode MHD waves and one associated with fast-mode waves. (Perpendicular MHD shocks are associated only with the fast/magnetosonic mode.) For the oblique fast-mode shock wave, the density increases and the flow speed decrease across the shock, as before. an oblique fast-mode shock; thus, the direction of  $\vec{B}$  must change across the shock front.

Many examples of shocks in space plasmas exist:

- 1. Collisionless fast-mode MHD shocks in the solar wind flow called planetary bow shocks have been observed by spacecraft at all the planets in the solar system except Pluto.
- 2. Shocks called interplanetary shocks have been observed in the solar wind. These are not associated with planets but with transient solar phenomena or with interaction of slow and fast "streams" in solar wind.
- 3. A shock called the heliosphere termination shock is thought to exist at the outer boundary of the heliosphere, where the solar wind runs up against the interstellar medium.
- 4. Slow-mode MHD shocks are thought to be present in the Earth's magnetotail.

# Curriculum Vitae



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