NONLINEAR PARTICLE ACCELERATION IN OBLIQUE SHOCKS

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ABSTRACT

The solution of the nonlinear diffusive shock acceleration problem, where the pressure of the nonthermal population is sufficient to modify the shock hydrodynamics, is widely recognized as a key to understanding particle acceleration in a variety of astrophysical environments. We have developed a Monte Carlo technique for self-consistently calculating the hydrodynamic structure of oblique, steady state shocks, together with the first-order Fermi acceleration process and associated nonthermal particle distributions. This is the first internally consistent treatment of modified shocks that includes cross-field diffusion of particles. Our method overcomes the injection problem faced by analytic descriptions of shock acceleration and the lack of adequate dynamic range and artificial suppression of cross-field diffusion faced by plasma simulations; it currently provides the most broad and versatile description of collisionless shocks undergoing efficient particle acceleration. We present solutions for plasma quantities and particle distributions upstream and downstream of shocks, illustrating the strong differences observed between nonlinear and test particle cases. It is found that, for strong scattering, there are only marginal differences in the injection efficiency and resultant spectra for two extreme scattering modes, namely large-angle scattering and pitch-angle diffusion, for a wide range of shock parameters, i.e., for nonperpendicular subluminal shocks with field obliquities less than or equal to 75° and de Hoffmann-Teller frame speeds much less than the speed of light.

Subject heading: acceleration of particles — cosmic rays — diffusion — hydrodynamics — shock waves

1. INTRODUCTION

The importance of shocks as generators of highly nonthermal particle distributions in heliospheric and astrophysical environments has been well documented in the literature (see, e.g., Axford 1981; Völk 1984; Blandford & Eichler 1987; Jones & Ellison 1991). While direct detections of high-energy particles are obtained via terrestrial observations of the cosmic-ray flux and spacecraft measurements of nonthermal ions in the solar neighborhood and in environs of planetary bow shocks and interplanetary travelling shocks, the existence of abundant nonthermal particle populations in a diversity of astrophysical locales can be inferred from the prominence of nonthermal radiation emitted by many cosmic objects. Understanding the details of shock acceleration is of critical importance since many such objects emit predominantly nonthermal radiation, and indeed some sources are observed only because they produce nonthermal particles (e.g., radio emission from supernova remnants and extragalactic jets). The first-order Fermi mechanism of diffusive shock acceleration is the most popular candidate for particle energization at astrophysical shocks. The test particle (i.e., linear) theory (Krymsky 1977; Axford, Leer, & Skadron 1977; Bell 1978; Blandford & Ostriker 1978) of this process is straightforward and yields the most important result, namely that a power law with a spectral index that is relatively insensitive to the ambient conditions is the natural product of collisionless shock acceleration.

The equally important question of the efficiency of the process can only be adequately addressed with a fully non-

linear (and therefore complex) calculation. The inherent efficiency of shock acceleration, which is evident in observations at Earth's bow shock (see, e.g., Ellison, Möbius, & Paschmann 1990b) and in modeling of plane-parallel (e.g., see Ellison & Eichler 1985; Ellison, Jones, & Reynolds 1990a) shocks, where the field is normal to the shock, and oblique shocks (see, e.g., Baring, Ellison, & Jones 1993; Ellison, Baring, & Jones 1995), implies that hydrodynamic feedback effects between the accelerated particles and the shock structure are very important and therefore essential to any complete description of the process. This has turned out to be a formidable task because of the wide range of spatial and energy scales that must be self-consistently included in a complete calculation. On the one hand, the microphysical plasma processes of the shock dissipation control injection from the thermal population, and on the other hand, the highest energy particles (extending to at least 10¹⁴ eV in the case of galactic cosmic rays) with extremely long diffusion lengths are dynamically significant in strong shocks and feedback on the shock structure. Ranges of interacting scales of many orders of magnitude must be described self-consistently.

Additional complications stem from the fact that the geometry of shocks, i.e., whether they are oblique or parallel, strongly affects the acceleration efficiency (see, e.g., Ellison et al. 1995), even though the test particle result is independent of the geometry. Observations indicate that interplanetary shocks, bow shocks (both planetary and from jets), the solar wind termination shock, and supernova remnant blast waves have a wide range of obliquities, thereby rendering considerations of shock geometry salient. It turns out that the angle between the upstream magnetic field and the shock normal, Θ_{Bn1} , is a decisive parameter in

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determining all aspects of the shock, including the ability to inject and accelerate particles, and therefore has obvious observational consequences. For instance, diffuse ions generated at quasi-parallel portions of Earth's bow shock differ radically in energy content, distribution function, etc., from field-aligned beams generated at quasi-perpendicular portions of the shock (see, e.g., Ipavich et al. 1988). Furthermore, the observed variation of radio intensity around the rim of shell-like supernova remnants may be the result of varying shock obliquity (see, e.g., Fulbright & Reynolds 1990), and the acceleration of the anomalous cosmic-ray component at the solar wind termination shock may depend on rapid acceleration rates obtained in highly oblique portions of the shock (Jokipii 1992). Unfortunately, in models that ignore the plasma microstructure as we do here, oblique shocks are more complicated and require additional parameters for a complete description than do parallel (i.e., $\Theta_{Bn1} = 0^{\circ}$) ones, primarily the degree of diffusion perpendicular to the mean ambient magnetic field direction.

In this paper we present our method for calculating the structure of steady state, collisionless shocks of arbitrary obliquity and with efficient particle injection and acceleration. The method, a computer simulation using Monte Carlo techniques, is an extension of our previous work on modified parallel shocks (see, e.g., Jones & Ellison 1991 and references therein), where we explored the properties of the nonlinear modified shock scenario, and test particle oblique shocks (Ellison et al. 1995; Baring, Ellison, & Jones 1993, 1995a), where we determined the dependence of acceleration efficiency on obliquity Θ_{Bn1} . These studies have been successfully applied to Active Magnetospheric Particle Tracer Explorer (AMPTE) observations near the parallel portion of Earth's bow shock (Ellison et al. 1990b), a high Mach number shock with strong modification by the accelerated ions, and measurements by Ulysses at highly oblique travelling interplanetary shocks in the heliosphere (Baring et al. 1995b, 1996), which generally have low Mach numbers and therefore are well modeled by linear test particle simulations. The impressive fits obtained to the spectral data (i.e., ion distribution functions) from each of these experiments underlines the importance of the Fermi mechanism and the value of the Monte Carlo technique. The present work represents the first self-consistent treatment of modified shocks that includes three-dimensional diffusion.

With the Monte Carlo simulation, we self-consistently determine the average flow speed and magnetic field structure across the shock under the influence of accelerated particles, maintaining constant particle, momentum, and energy fluxes at all positions from far upstream to far downstream of the shock. Particles are injected upstream of the shock, propagated, and diffused in the shock environs until they eventually leave the system. We calculate their orbits exactly as in the works of Decker (1988), Begelman & Kirk (1990), Ostrowski (1991), and our recent test particle treatment (Ellison et al. 1995) and make no assumption relating to the particle magnetic moment. Our method does not self-consistently calculate the complex plasma processes responsible for dissipation but instead postulates that these processes can be adequately described with a simple elastic scattering relation that is assumed to be valid for all particle energies; thermal and nonthermal particles are treated identically. This simplification sacrifices the details of waveparticle interactions but permits simultaneous description of the thermal plasma and the particle injection and acceleration to the high energies associated with space plasma shocks, thereby satisfying the aforementioned goal of broad dynamic range. Cross-field diffusion is included via a parametric description but is fully three-dimensional, in contrast to hybrid or full plasma simulations with one or two ignorable dimensions that suffer from artificial suppression of cross-field diffusion (see, e.g., Jokipii, Giacalone, & Kóta 1993). Simulation output includes the ion distribution function at all relevant positions in the shocked flow for a range of obliquities and Mach numbers.

Results are compared (in § 4) for two extreme scattering modes, namely large-angle scattering (LAS), where the direction of a particle is isotropized in a single scattering event, and pitch-angle diffusion (PAD), where small changes in the angle a particle's momentum makes with the local magnetic field occur at each time step. The former of these extremes mimics particle motion in highly turbulent fields, while the latter is usually implemented in analytic treatments of Fermi acceleration (see, e.g., Kirk & Schneider 1987, but see also the Monte Carlo work of Ostrowski 1991). We find that in our application to nonrelativistic shocks, the choice of scattering mode is largely immaterial to the resultant distributions as long as scattering is reasonably strong; we expect this not to be so for weak scattering or for relativistic shocks, where the modes generate vastly different particle anisotropies. We also compare nonlinear (§ 4.2) results with test particle results where the nonthermal particles do not modify a discontinuous shock (§ 4.1), finding that, as in our earlier work on plane-parallel shocks, some spectral curvature arises in high Mach number shocks in which a large fraction of the partial pressure resides in the nonthermal population. An outline of the Monte Carlo method is given in § 2, followed in § 3 by flux conservation considerations and the associated scheme for iterative determination of the modified shock flow and field profiles. The spectral and flux results comprise § 4, culminating in a presentation of acceleration efficiencies and discussion of the results.

2. THE MONTE CARLO METHOD

The Monte Carlo technique for describing particle acceleration at plane shocks has been described in previous papers (see, e.g., Ellison et al. 1990a; Jones & Ellison 1991; Baring et al. 1993; Ellison et al. 1995) and is essentially a kinematic model that closely follows Bell's (1978) approach to diffusive acceleration. The simulation follows individual particles as they traverse a background "plasma" consisting of an average bulk flow and magnetic field; the flow velocity and magnetic field consist of a grid of values from far upstream to far downstream with a subshock positioned at x = 0. Our subshock is a substructure of the overall shock, defining the conventional boundary between (infinite) upstream and downstream regions. Strictly, it should be no sharper than the smallest diffusion scale (i.e., the gyroradius of thermal particles); however, in most cases, we require it to be abrupt for the purposes of expedience in the simulation. Particles are injected far upstream of the shock with a thermal distribution at temperature T_1 , mimicking, for example, solar wind ions (as in applications to Earth's bow shock) and are allowed to convect in the flow and scatter, crossing the shock a few or many times before they eventually leave the system either far downstream or beyond an upstream free escape boundary (FEB). They are moved one at a time according to a prescribed scattering law, defined below, in a test particle fashion until they exit the simulation. In cases in which efficient acceleration arises, feedback of the accelerated population leads to significant smoothing of the shock profile and heating of particles occurs in the foreshock region; discussion of such nonlinear aspects of the simulation are deferred to § 3 below.

Following our previous treatments of oblique shocks (Baring et al. 1993; Ellison et al. 1995), particle convection is performed in the de Hoffmann-Teller (HT) frame (de Hoffmann & Teller 1950), a frame in which the shock is stationary, the fluid flow u is everywhere parallel to the local field **B**, and the electric field is $\mathbf{u} \times \mathbf{B} = 0$ everywhere. The HT frame of reference is therefore particularly convenient because of the associated absence of drift electric fields: particle trajectories are then simple gyrohelices, and the description of convection is elementary. Furthermore, it follows from the mere existence of an HT frame that the so-called shock drift mechanism is inseparable from, and intrinsically part of, the Fermi acceleration process (see, e.g., Drury 1983; Jones & Ellison 1991) and is therefore automatically included in our Monte Carlo technique since particle motion is followed in the HT frame.

While field and flow directions in the HT frame are uniquely defined downstream of the shock, the nonlinear nature of this work yields a spatial variation of u and Bbecause of the compressive effects of the accelerated population. This variation is accommodated using a grid zone structure that was implemented in many earlier versions of the Monte Carlo technique; each zone contains uniform field and flow, with discontinuities at the boundaries satisfying the Rankine-Hugoniot conditions discussed in § 3 below. The grid zone boundaries therefore mimic minishocks, with the subshock defining a particular grid boundary; a depiction of this grid structure is given in Baring, Ellison, & Jones (1992). The spatial resolution of the grid can be adapted at will, but in our applications, we require it to be finer at some distance upstream than the typical mean free path of particles that penetrate to that distance from the shock. Note that the ability to define (for example, via the Rankine-Hugoniot conditions) an HT frame with $\boldsymbol{u} \times \boldsymbol{B} = 0$ on both sides of a grid point implies, by spatial extension, that the HT frame is uniquely defined throughout the flow, regardless of flow and field compression and deflection upstream. In addition, note that even though the $u \times B$ electric field is transformed away by going to the HT frame, charge separation electric fields are not, and these have not been included in our model, being beyond the scope of the present work.

While particle transport is monitored in the HT frame, all measured quantities such as particle distributions and momentum and energy fluxes are output in the normal incidence frame (NIF), which is the frame in which the shock is also stationary but which is defined such that the flow far upstream (i.e., where it is uniform to infinity) is normal to the shock plane. A simple velocity boost with a speed of $v_{\rm HT} = u_1 \tan \Theta_{Bn1}$ parallel to the shock front effects transformation between the NIF and HT frames, where Θ_{Bn1} is the far upstream angle the magnetic field makes with the shock normal and u_1 is the far upstream flow speed in the NIF. Note that hereafter, the index "1" will indicate far upstream values and the index "2" will indicate far downstream values well away from the smooth shock transition.

A depiction of the NIF geometry is given in Figure 1 for the specific case of unmodified shocks; modified shock geometry extends this to include piecewise increments of u and B. In the normal incidence frame, the -x-axis defines the shock normal, and the senses of the other axes are as in Figure 1. The results of this paper are restricted to highly subluminal cases where $v_{\text{HT}} \ll c$, the speed of light, since our Monte Carlo technique has not yet been generalized to include relativistic effects in oblique shocks.

The simulation is an orbit code, where particle propagation is performed by following the gyromotions exactly, as in the test particle work of Ellison et al. (1995) and a diversity of works in the literature (see, e.g., Decker 1988; Begelman & Kirk 1990; Ostrowski 1991; Takahara & Terasawa 1991). The position of particles is incrementally updated on a timescale δt , which is a small fraction of a gyroperiod, i.e., $\delta t \ll \tau_g = mc/(QeB)$, where m and Q are the particle's mass and charge number respectively, and e is the electronic charge. A particle in a particular grid zone is moved in a helical orbit determined by the magnetic field and bulk flow velocity for that grid position.

2.1. Particle Scattering

Having outlined the procedure for convection, here we describe our prescription for particle scattering, which is somewhat more involved. After each time step δt , a determination of whether the particle should "scatter" or not is made using a scattering probability $P_{\text{scat}} = \delta t/t_c$, where the collision time, t_c , is given by λ/v , λ is the mean free path, and $v \ll c$ is the particle speed, both measured in the local fluid frame. This prescription yields an exponential pathlength distribution. The scatterings, presumably off magnetic irregularities in the flow, are assumed to be elastic in the local plasma frame so that monotonic energy gains natu-



FIG. 1.—Geometry of a discontinuous plane shock in the normal incidence frame (NIF), the frame where particle distributions and fluxes are output from the simulation. The shock lies in the y-z plane, and all quantities vary only in x. The geometry of the "smooth" shock is similar except that the magnetic field and flow make many small kinks instead of one large one, i.e., the profiles consist of a sequence of connected pieces like this depiction.

rally arise as a particle diffuses back and forth across the shock because of the converging nature of the flow. The assumption of elasticity of scattering is suitable when the particle speed far exceeds the Alfvén speed; it is therefore appropriate for all shocks with not very low Alfvénic Mach numbers. It proves convenient to scale the mean free path by the gyroradius, introducing a model parameter η that is the ratio of the two quantities (following Jokipii 1987; Ellison et al. 1995):

$$\lambda = \eta r_g \quad \text{or} \quad \kappa_{\parallel} = \frac{1}{3} \eta r_g v , \qquad (1)$$

where κ_{\parallel} is the diffusion coefficient parallel to the local magnetic field. It follows that the collision time satisfies

$$t_c = \frac{\lambda}{v} = \frac{\eta r_g}{v} = \eta \, \frac{mc}{QeB} \,. \tag{2}$$

Generally, η is a function of energy; however, in this paper, it is assumed to be a constant independent of position and energy (also following Jokipii 1987). For this choice, the collision time is independent of particle energy, a convenient simplification that can be easily generalized to some other dependence of λ on r_g (see Ellison et al. 1990b). Note also that λ is hence implicitly inversely proportional to *B*.

The assumed constancy of η is the most important approximation we make, since all of the complicated plasma physics of wave-particle interactions is incorporated in equation (1). Convenience aside, there are sound reasons for choosing this simple relation. First of all, as long as electrostatic effects are neglected (they are omitted from our treatment), the gyroradius is the fundamental scale length of a particle at a particular energy, and the mean free path can be expected to be some function of this parameter. Second, if the plasma is strongly turbulent with $\delta B/B \sim 1$, as is generally observed in space plasmas, the large-scale structures in the magnetic field will mirror particles effectively on gyroradii scales (i.e., for $\eta \approx 1$, the Bohm diffusion limit; Zachary 1987). Third, and most important, spacecraft observations suggest that $\lambda \propto r_g$ in the self-generated turbulence near Earth's bow shock (see, e.g., Ellison et al. 1990b). Fourth, hybrid plasma simulation results also suggest that the mean free path is a moderately increasing function of r_a (Giacalone, Burgess, & Schwartz 1992; Ellison et al. 1993). Note that while the exact form for λ will surely have quantitative effects on the injection rate and all other shock characteristics, the most important qualitative effects should be well modeled as long as a strongly energy dependent diffusion coefficient is used. Employing a realistic κ_{\parallel} with a strong energy dependence is essential because of the intrinsic efficiency of shock acceleration. If κ_{\parallel} is indeed energy dependent, the highest energy particles with large fractions of energy and pressure have very different scales from thermal particles, which leads to the spectral curvature that appears in the simulated distributions (see § 4).

The simulation employs two complementary types of scattering modes, namely large-angle scattering and pitchangle diffusion. For each mode, elasticity of scattering is imposed, which amounts to neglecting any recoil effects of wave production on the particles and hence that the background scattering centers (i.e., magnetic irregularities) are frozen in the plasma. This approximation is generally quite appropriate but becomes less accurate for low Afvénic Mach numbers when the flow speed does not far exceed the Alfvén wave speed. In large-angle scattering (LAS), a partiVol. 473

cle's direction is randomized in a single scattering event (on a timescale of t_c) and the new direction is made isotropic in the local plasma frame. Such quasi-isotropic scattering is adopted in most of our earlier simulation work (e.g., see Jones & Ellison 1991; Baring et al. 1993; Ellison et al. 1995) and is intended to mimic the effect of large-amplitude field turbulence on particle motions. Such turbulence is present in both plasma simulations (see, e.g., Quest 1988; Burgess 1989; Winske et al. 1990) and observations of shocks in the heliosphere (see, e.g., Hoppe et al. 1981).

The second scattering mode we employ is pitch-angle diffusion (PAD), as used in the diverse works of Decker & Vlahos (1985), Decker (1988), Kirk & Schneider (1987), and Ostrowski (1988, 1991). In this mode, the direction of the velocity vector v is changed by a small amount after each time step, δt , rendering the scattering process more "continuous" than large-angle collisions and more appropriate to physical systems with small levels of field turbulence. Here we adopt the procedure detailed in Ellison et al. (1990a) for determining the maximum amount the pitch angle $\hat{\theta}_B = \arccos \{ \boldsymbol{v} \cdot \boldsymbol{B} / |\boldsymbol{v}| |\boldsymbol{B}| \}$ can change after each δt ; our procedure is summarized in the Appendix. A comparison of the simulation results for these two modes is one goal of this paper, motivated by an expectation that they could, in principle, produce different injection efficiencies at modified shocks. This expectation is partly based on the spectral differences observed between LAS and PAD applications to unmodified relativistic shocks (see, e.g., Ellison et al. 1990a), where the two modes generate significantly different particle anisotropies; distribution anisotropies are indeed relevant to the injection problem considered here.

As a particle convects, the simulation tracks both its position and the position of its gyrocenter. After a scattering occurs and a new direction is obtained for its velocity vector, a new gyrocenter is calculated. This shift of the gyrocenter means the particle is now gyrating around a different field line and diffusion across the field has occurred; the new field line is within $2r_g$ of the one the particle was circling before the scattering. Such cross-field diffusion is an integral part of diffusive acceleration at oblique shocks (see, e.g., Jokipii 1987; Ellison et al. 1995), and its presence is required in the Monte Carlo simulation in order to match spacecraft observations of particle spectra associated with interplanetary shocks (Baring et al. 1995b, 1996; see also Jones & Kang 1995). Ellison et al. (1995) showed that this scheme for cross-field diffusion together with the assumption contained in equation (1) is equivalent to a kinetic theory description of diffusion (see, e.g., Axford 1965; Forman, Jokipii, & Owens 1974), where the diffusion coefficients perpendicular to (κ_{\perp}) and parallel to (κ_{\parallel}) the field are related via $\kappa_{\perp} =$ $\kappa_{\parallel}/(1+\eta^2)$. The parameter η in equation (1) then clearly determines the strength of the scattering and when $\eta \sim 1$, $\kappa_{\perp} \sim \kappa_{\parallel}$, the so-called Bohm limit, where particles diffuse across the magnetic field as quickly as they move along it. The properties of highly oblique and quasi-parallel shocks tend to merge when the scattering is strong.

2.2. Grid Zone, Free Escape, and Downstream Return Boundaries

When a particle crosses a grid zone boundary, the values of the bulk flow velocity and the magnetic field (both magnitude and direction for these vector quantities) change, and a new gyroradius, gyrocenter, and phase in the gyro-orbit are determined, as outlined in the Appendix. The particle

then acquires a new gyromotion with subsequent convection along the new field direction. At a crossing of a grid zone boundary, we adopt the standard requirement (e.g., see Terasawa 1979; Decker 1988; Begelman & Kirk 1990) in orbit calculations that the momentum vector of the particle is conserved in the de Hoffmann-Teller frame, since there is no electric field in the shock layer in this frame. While this implies conservation of energy in the HT frame (i.e., between scatterings), particle energies do change at the discontinuity in the NIF (see, e.g., Toptyghin 1980) because of the presence of drift electric fields, a manifestation of the transformation between frames. This transmission criterion differs from the imposition of magnetic moment conservation that was made in earlier applications of our Monte Carlo technique (see, e.g., Baring et al. 1993); in the present paper, we make no assumption concerning the magnetic moment of a particle at a grid point or anywhere else. Particles may of course "reflect" at any zone boundary or be transmitted depending on their phase and pitch angle after a number of gyrations in the vicinity of the boundary.

There are two limiting boundaries to the simulation region: the free escape boundary (FEB) and the downstream return boundary. Our introduction of an upstream FEB facilitates modeling of the finite extent, for example through geometrical curvature, of real shocks. Escape is naturally expected in real systems, since the region of influence of a shock on its environs is finite, and the level of shock-generated turbulence diminishes to background levels at sufficient distances from the shock. An escape boundary is most relevant to the upstream region (1) because the direction of convection renders the downstream region more spatially uniform and (2) because the upstream region is usually on the convex side of the shock (e.g., supernova remnant shocks, the Earth's bow shock), although particles can escape from the downstream side as well. The inclusion of such a free escape boundary is also motivated on theoretical grounds. The fundamental point is that for Fermi acceleration in steady state shocks, escape must occur for Mach numbers above some critical value. This has been fully documented (see, e.g., Eichler 1984, 1985; Ellison & Eichler 1984; Jones & Ellison 1991), where it is observed that within the context of the nonlinear acceleration model, the Fermi acceleration/hydrodynamics coupling becomes unstable for shocks of Mach numbers above a few and leads to singularities in the energy density when particle escape is suppressed. Finite solutions are achievable when an upstream FEB is introduced, since its presence causes the acceleration process to truncate at the highest energies. In the case in which the diffusion coefficient increases with energy, the FEB produces a distribution that falls off approximately exponentially at an energy at which the upstream diffusion length is on the order of the distance from the FEB to the shock. In the simulation, particles are removed just before they scatter for the first time on the upstream side of the FEB; this choice leads to a spatial smearing of the effects of the FEB on the scale length of the mean free path of the escaping particles, i.e., on length scales comparable to the distance d_{FEB} between the FEB and the shock.

In the results presented here, the FEB is chosen close enough to the shock to guarantee that all particles in the simulation remain nonrelativistic; the domain of acceleration to relativistic energies and also relativistic shock scenarios are deferred to future work. The dynamical consequences of the FEB are discussed in detail in § 4 below.

While the upstream region in the simulation is finite, delimited with a FEB, we model an infinite downstream region with a probability of return calculation beyond a downstream return boundary (DRB); this spatial border renders the simulation finite in time. Beyond the DRB, which is maintained more than a scattering length downstream of the shock, the spatial diffusion properties are treated using appropriate statistical probabilities. If the position of a particle (as opposed to its guiding center) is followed, then the probability of return to the upstream side of the DRB assumes a simple form. If the flow is uniform with a component of velocity u_{x2} perpendicular to the DRB (in our case, this direction is also perpendicular to the shock plane) and particles of speed v_F in the frame of the flowing plasma are also isotropic in that fluid frame, then the probability, P_{ret} , that a particle which crosses some arbitrary y-z plane will return to the upstream side of that plane, is

$$P_{\rm ret} = \left(\frac{v_F - u_{x2}}{v_F + u_{x2}}\right)^2 \,. \tag{3}$$

While this calculation has been done many times (see, e.g., Bell 1978; Drury 1983; Jones & Ellison 1991; Ellison et al. 1995), we emphasize that equation (3) is fully relativistic (Peacock 1981) and holds regardless of the orientation of the magnetic field or the flow. The principal requirement for the validity of equation (3) is that the particles are isotropic in the local fluid frame, a condition that is satisfied since the DRB is at least a scattering length downstream of the shock. Hence, while equation (3) can be used downstream where the flow is uniform for any $v_F \gtrsim u_{x2}$, it cannot be used at the shock where the flow speed changes unless $u_{x2} \ll v_F$. The particle speed, v_F , must also remain constant during the time a particle spends downstream from the y-z plane, a natural consequence of our elastic scattering assumption. The decision of return (or otherwise) is made via a random number generator. Particles that do return must be injected back across the y-z plane with properly flux-weighted xcomponents of velocity, pitch angles, and phases. The determination of these, along with a detailed derivation of equation (3), are given in the Appendix. Note that the DRB is not only a feature of our Monte Carlo simulation but is also used in hybrid plasma simulations of shocks (Bennett & Ellison 1995).

3. FLUX CONSERVATION RELATIONS AND SHOCK MODIFICATION

Before presenting the results of our modified shock simulations, it is instructive to review the elements of nonlinear shock hydrodynamics and our procedure for determining the fluid flow and magnetic field spatial profiles that simultaneously conserve all relevant fluxes and are also selfconsistent products of the Fermi acceleration mechanism.

3.1. Flux Conservation Relations

The starting point for these considerations is the wellknown one-dimensional, steady state, magnetohydrodynamic conservation relations (i.e., the Rankine-Hugoniot [R-H] jump conditions) for an infinite, plane shock lying in the y-z plane (see the geometry in Fig. 1). Variations of all quantities occur only in the x-direction, and these equations are written in the normal-incidence frame (NIF). The notation is that of Decker (1988), with the square brackets representing differences between quantities far upstream (with the "1" subscript) and downstream (with the "2" subscript) of the shock; however, the origin of the forms used here is based on the presentation of Boyd & Sanderson (1969, p. 56). For a magnetic field strength of B, if u is the bulk speed of the plasma, the purely electromagnetic equations (i.e., Maxwell's equations) are

$$[B_x]_1^2 = 0 , (4)$$

which defines a divergenceless magnetic field (remember that our system has $\partial B_y/\partial y = 0 = \partial B_z/\partial z$), and

$$[u_z B_x - u_x B_z]_1^2 = 0, (5)$$

which expresses (since $c\nabla \times E = -\partial B/\partial t = 0$) the uniformity of the tangential electric field across the shock. The hydrodynamic equations are as follows: the mass flux equation corresponding to the x-direction is

$$[\rho u_x]_1^2 = 0 , (6)$$

where ρ is the mass density; the equations for the flux in the x-direction of the x and z components of momentum are

$$\left[\rho u_x^2 + P_{xx} + \frac{B_z^2}{8\pi}\right]_1^2 = 0 , \qquad (7)$$

and

$$\left[\rho u_{x}u_{z} + P_{xz} - \frac{B_{x}B_{z}}{4\pi}\right]_{1}^{2} = 0, \qquad (8)$$

respectively, where P_{xx} and P_{xz} are the appropriate components of the pressure tensor. Finally, the energy flux in the x-direction satisfies

$$\left[\frac{\gamma}{\gamma - 1} P_{xx} u_x + P_{xz} \left\{ u_z + \frac{u_x}{3(\gamma - 1)} \left(\frac{2B_x}{B_z} + \frac{B_z}{B_x} \right) \right\} + \frac{1}{2} \rho u_x^3 + \frac{1}{2} \rho u_x u_z^2 + \frac{u_x B_z^2}{4\pi} - \frac{u_z B_x B_z}{4\pi} + Q_{esc} \right]_1^2 = 0.$$
(9)

Here γ is the ratio of specific heats, which enters via the thermal contribution to the energy density using the equation of state; we set this equal to 5/3 in this paper, since only nonrelativistic particles appear in the simulation results presented. Equations (7)–(9) neglect so-called gradient terms that are spatial diffusion contributions that arise from non-uniformity of the fluid flow and magnetic field profiles. Note also that equations (7), (8), and (9) approximate the respective parallel shock relations for high Alfvénic Mach numbers (i.e., where the field is dynamically unimportant), whereas equation (5) remains important regardless of the Mach number.

In equation (9), we have added the term, Q_{esc} , to model the escape of particles at an upstream free escape boundary (FEB). As mentioned above, a FEB causes the acceleration process to truncate as particles leave the system, producing important dynamical effects since the escaping energy, and therefore pressure, results in an increase in the compression ratio of the shock (see Ellison et al. 1990a for a discussion of the effects of such a term in the R-H relations). The escaping energy flux, Q_{esc} , is taken to be constant for the far downstream region and zero for the region far upstream (i.e., several mean free paths) of the FEB and varies most rapidly in the neighborhood of the FEB. We assume that the concurrent escaping momentum and mass fluxes are small and neglect them in equations (6), (7), and (8). This is a good approximation if the particles that escape have speeds such that $v_{\rm esc} \ge u_{x1}$ (see Ellison 1985), a situation that is always realized in the simulation results presented here.

The appearance of different components of the pressure tensor in the Rankine-Hugoniot relations is requisite for the Monte Carlo simulation since we do not assume that particles are isotropic in any frame. Normally, implementations of the conservation equations in astrophysical or heliospheric applications (see, e.g., Decker 1988) are restricted to scenarios in which the plasma is isotropic in the local fluid frame, in which case $P_{xx} = P_{yy} = P_{zz} = P$ and the offdiagonal terms of the pressure tensor are zero. However, our system generates anisotropic plasma in all frames of reference because of the nonuniformity of the flow *combined* with the self-consistently determined Fermi acceleration of the particles. In this paper, for the sake of simplicity, we assume that the plasma is gyrotropic but anisotropic in the local fluid frame in the flux equations.

When an isotropic population of particles is convected across a velocity discontinuity and then subjected to isotropic scattering, compression of the plasma is close to, but not perfectly, gyrotropic: asymmetric phase sampling at the discontinuity yields nonuniform phase distributions prior to scattering. Plasma isotropy in the new local fluid frame is attained only after many scattering lengths; in fact, adjustment to true isotropy is never achieved in our nonlinear Monte Carlo treatment because the scale length of velocity (and directional) changes in the fluid flow is always comparable to the mean free path of the particles comprising the flow. Gyrotropy is a good approximation that is also expedient because it yields a diagonal pressure tensor P_{ii} in the de Hoffman-Teller and fluid frames for coordinate systems with one axis aligned along the magnetic field; since the diagonal components generally differ, oblique shocks lead to nonzero off-diagonal components: $P_{xz} = P_{zx} \neq 0$. A discussion of the generation of such terms is presented in the Appendix, specifically focusing on the details of the derivation of the pressure terms of the energy flux in equation (9); there the coefficient of P_{xz} is alternatively expressed in terms of pressure components parallel to and orthogonal to the local field. Note that nonzero $P_{xy} = P_{yx}$ also arise in hydrogenic plasma flows in conjunction with out-of-theplane components of the magnetic field (Jones & Ellison 1987, 1991); such off-diagonal terms apply only to quantities in the y-direction and therefore are irrelevant to the considerations of this paper.

Note that in all of the examples described below, we have expediently set the electron temperature equal to zero. We assume, as is generally done in the literature, that the ions dominate the shock structure and that the addition of electrons has little effect on the dynamics other than changing the Mach number. This follows from the fact that electrons carry little momentum compared to protons. For most acceleration models, electrons can be treated as test particles in the ion-determined flow. A finite temperature of electrons and their heating by the shock can be modeled in a simple way with our procedure by treating the electrons as a fluid and is necessary when fitting spacecraft observations; this was done in applications to Earth's bow shock (Ellison et al. 1990b) and interplanetary shocks (Baring et al. 1996). In such heliospheric applications, shocks put far more energy into nonthermal ions than electrons, so the role of electrons is largely peripheral. In astrophysical settings outside the solar system, the presence of nonthermal electrons is generally inferred by the observations while the existence of accompanying accelerated ion populations is often unknown. It is unclear whether or not in such sources as supernova remnants (SNRs), active galaxies etc., electrons carry a sizable fraction of the total energy budget, though efficiency considerations argue in favor of this. Models of electron injection and acceleration in shocks are difficult to develop because the electron diffusion depends on the details of the microphysics. The Monte Carlo technique can be adapted to treat Fermi acceleration of electrons if it is assumed that they follow some simple prescription of scattering such as in equation (1); this was successfully performed in Ellison & Reynolds (1991) for plane-parallel shocks, with interesting observational consequences in SNRs. This somewhat involved extension of the Monte Carlo technique in oblique shock scenarios is beyond the scope of the present paper and is deferred to future work. Notwithstanding, the division of energy between electrons and ions in shock acceleration remains an important unresolved question.

3.2. Flux Scalings and Formalism

The flux equations are used in the simulation in dimensionless form, scaling by relevant upstream quantities. In the NIF, the far upstream flow is taken along the shock normal, i.e., $u_{z1} = 0$. We define the flow velocity $u_1 \equiv u_{1x}$, the magnitude of the far upstream magnetic field $B_1 \equiv (B_{1x}^2 + B_{1z}^2)^{1/2}$, and a far upstream plasma density ρ_1 . These specify a far upstream Alfvénic Mach number: $M_{A1} = u_1/v_{A1}$ or $M_{A1}^2 = (4\pi\rho_1 u_1^2)/B_1^2$, where the Alfvén speed is $v_{A1} = B_1/(4\pi\rho_1)^{1/2}$, and a far upstream sonic Mach number, $M_{S1}^2 = \rho_1 u_1^2/(\gamma P_1)$, where $P_1 = n_1 k_B T_1$ is the far upstream (isotropic) pressure. Here n_1 and T_1 are the number density and temperature far upstream, and k_B is Boltzmann's constant. These upstream parameters, along with Θ_{Bn1} , define the key input for the simulation runs. Using these definitions, one can write equations (5) and (7)–(9) in a dimensionless form at any position x:

$$u'_{z}(x)B'_{x1} - u'_{x}(x)B'_{z}(x) = F'_{uB}, \qquad (10)$$

defines the uniformity of tangential electric field,

$$u'_{x}(x) + P'_{xx}(x) + \frac{B'_{z}(x)}{2M^{2}_{A1}} = F'_{xx1}$$
, (11)

and

$$u'_{z}(x) + P'_{xz}(x) - \frac{B'_{x1}B'_{z}(x)}{M^{2}_{A1}} = F'_{xz1} , \qquad (12)$$

define the momentum flux equations, and

1

$$\frac{\gamma}{\gamma - 1} P'_{xx}(x)u'_{x}(x) + P'_{xz}(x) \\ \times \left\{ u'_{z}(x) + \frac{u'_{x}(x)}{3(\gamma - 1)} \left[\frac{2B'_{x1}}{B'_{z}(x)} + \frac{B'_{z}(x)}{B'_{x1}} \right] \right\} \\ + \frac{1}{2} u'^{2}_{x}(x) + \frac{1}{2} u'^{2}_{z}(x) + \frac{B'_{z}(x)}{M^{2}_{A1}} \\ \times \left[u'_{x}(x)B'_{z}(x) - u'_{z}(x)B'_{x1} \right] + Q'_{esc} = F'_{en1} , \qquad (13)$$

rearranges the energy flux equation. All primed quantities are dimensionless, using the notation $u' = u/u_1$, $B' = B/B_1$, $P' = P/(\rho_1 u_1^2)$, and $Q'_{esc} = Q_{esc}/(\rho_1 u_1^3)$. Note that $\gamma = 5/3$ is a

constant throughout the flow for the nonrelativistic applications here. The constancy of the x-component of magnetic field has been used to substitute $B'_x(x) = B'_{x1}$, and we have also used mass flux conservation

$$\rho(x)u_x(x) = \rho_1 u_1 = \text{constant} , \qquad (14)$$

in these equations. As mentioned above, the escaping momentum and mass fluxes are of progressively smaller orders in u_{x1}/v_{esc} than Q'_{esc} and therefore are neglected. The far upstream fluxes on the right-hand sides of equations (10)–(13) are constants determined by the input shock parameters:

$$F_{uB}^{\prime} = -B_{z1}^{\prime},$$

$$F_{xx1}^{\prime} = 1 + P_{1}^{\prime} + \frac{B_{z1}^{\prime 2}}{2M_{A1}^{2}},$$

$$F_{xz1}^{\prime} = -\frac{B_{x1}^{\prime}B_{z1}^{\prime}}{M_{A1}^{2}},$$

$$F_{en1}^{\prime} = \frac{\gamma}{\gamma - 1}P_{1}^{\prime} + \frac{1}{2} + \frac{B_{z1}^{\prime 2}}{M_{A1}^{2}}.$$
(15)

If Q'_{esc} and P'_{xz} are both assumed to be zero at all x, the four unknowns in equations (10)–(13), $u'_x(x)$, $u'_z(x)$, $P'_{xx}(x)$, and $B'_{z}(x)$, can be obtained at every position x. This is just the standard situation of a discontinuous shock, and these Rankine-Hugoniot relations are analytically solvable (e.g., see Decker 1988) for the shock compression ratio, $r \equiv$ u_1/u_{x^2} . However, in the modified collisionless shocks considered here, the nonthermal component of the particle distribution that is generated by particles crossing the shock more than once contributes significantly to the total pressure of the system, and $Q'_{\rm esc}$ will not, in general, be zero. In fact, Q'_{esc} will have different values at various locations and cannot be determined before the shock structure is known, which makes a direct solution of equations (10)-(13) impossible; this is the inherent nonlinearity in the problem even if isotropy is assumed, defined by the coupling between the acceleration process and the flow hydrodynamics.

In our approach, we iterate to achieve a solution for the velocity and field shock profiles by varying $u'_x(x)$, $u'_z(x)$, $B'_z(x)$, and the overall compression ratio for successive simulation runs (each accelerating particles and generating non-thermal distributions) until equations (10)–(12) are satisfied at every x. The overall compression ratio depends on Q'_{esc} far downstream from the shock and is determined by our solution. When this value is consistent with equation (13), a complete solution to the nonlinear acceleration problem is obtained, which satisfies equations (4)–(9) at all positions. The details of the iterative procedure follow.

3.3. Iteration of the Shock Profile

The iteration of the shock profile is done in two stages. We first choose the overall compression ratio (normally the R-H value for the first iteration), and, using this ratio, we iterate the *shape* of the profile. As individual particles move through the shock, the momentum and energy fluxes are calculated at each grid zone boundary. We therefore obtain the quantity

$$F'_{xx}(x) = u'_x(x) + P'_{xx}(x) + \frac{B'_z(x)}{2M_{A1}^2}$$
(16)

at each boundary, where $u'_x(x)$ and $B'_z(x)$ are the current values for the shock structure. From this we compute the



pressure $P'_{xx}(x)$ and calculate a new x-component of the flow speed from equation (11),

$$u_x^{\prime N}(x) = F_{xx1}' - P_{xx}'(x) - \frac{B_z^{\prime 2}(x)}{2M_{A1}^2}$$
(17)

such that the momentum flux will equal the constant far upstream value, F'_{xx1} , at all x. Replacing $u'_x(x)$ with $u'^N(x)$, we solve equations (10) and (12) for new values of $u'_z(x)$ and $B'_z(x)$. To speed convergence, before running the next iteration, we smooth this new profile, force it to be monotonic, average it with the previous profile, and scale the profile by setting values of the x-component of flow to u_{x2} for $x > 1\lambda_0$ and the far upstream value to u_{1x} . Since no wave physics is employed in our description, we do not attempt to model anything other than a monotonic decrease in flow speed and a monotonic increase in the magnitude and obliquity of **B** from upstream to downstream. Alternatively, we can calculate both $P'_{xx}(x)$ and $P'_{xz}(x)$ in the simulation and obtain the new prediction for $u'^N_x(x)$ from equation (13), but in either case, our procedure rapidly and stably converges.

With this new shock profile, we repeat the simulation by again injecting particles far upstream from the shock and propagating them until they leave at either the FEB or the probability of return plane. Our algorithm converges rapidly (within a few steps: see the examples in \S 4 below) to values of $u'_x(x)$, $u'_z(x)$, and $B'_z(x)$, which no longer change significantly with subsequent iterations. However, in general, this profile will not simultaneously conserve momentum and energy fluxes unless a compression ratio consistent with the escaping energy flux Q_{esc} has been chosen. The second stage of the iteration process is to choose successively new overall compression ratios (larger than the R-H value), each time repeating the iteration of the profile shape, and continue until the momentum fluxes and the energy flux (with $Q'_{\rm esc}$ added) are constant everywhere. Thus, within statistical limits, a shock profile and overall compression ratio that are consistent with the Fermi acceleration process are obtained. While we have no formal proof of the uniqueness of our solution, we have confirmed in a large number of examples that the final shock structure, for a given set of far upstream parameters, is independent of

state and in plane geometry, and several parameters control the dissipative processes as well as the injection from thermal energies into the Fermi acceleration mechanism. These far upstream parameters include the magnetic field strength, B_1 , the obliquity, Θ_{Bn1} , the temperature, T_1 , the number density, n_1 , and the shock speed, u_1 , all of which are determined by the ambient upstream conditions and can, in principle, be determined by observations of a given physical system. The size of the acceleration region is also an observable (for example, the radius of a supernova remnant shock), and we model it using the distance d_{FEB} between the upstream free escape boundary and the shock. However, the "size" of the shock in units of mean free paths is very important, and this will depend on the scattering law we assume. This requires the introduction of another parameter, η , the ratio of the mean free path to the gyroradius, via equation (1). The value of η , which determines the amount of cross-field diffusion, depends on the highly complex plasma interactions that occur in the shock environs; the prescription in equation (1) is a simple but insightful way to model these plasma processes.

Another "variable" results from the inclusion of two extreme modes of scattering, namely large-angle scattering (LAS) and pitch-angle diffusion (PAD). While more complicated scattering models can be used, we believe these contain the essential physics of plane shocks and yield important information on the nonlinear processes linking shock structure and particle acceleration. The type of scattering we employ and η are free parameters and cannot be determined in our model except by comparison with observations of space plasma shocks or three-dimensional plasma simulations. Hence (replacing B_1 and T_1 with M_{A1} and M_{S1}), there are seven parameters in our model: M_{A1} , M_{S1} , n_1 , Θ_{Bn1} , u_1 , d_{FEB} , and η , together with the choice of the type of scattering (either LAS or PAD). In all of the following examples, we use a shock speed of $u_1 = 500$ km s⁻¹ and a far upstream number density of $n_1 = 1$ cm⁻³, which define physical scales for our system that are more or less appropriate for astrophysical shocks. The spatial scales of the results presented here are all in units of the "lowenergy mean free path " λ_0 , which is defined as the mean free path (see eq. [1]) of a proton with speed u_1 in the upstream magnetic field, i.e., $\lambda_0 = \eta m_p u_1 c/(eB_1)$, where $\eta ~(\geq 1)$ remains an adjustable parameter for each simulation run.

4.1. Test Particle Examples

The simplest acceleration results obtainable from the Monte Carlo simulation are for test particle cases in which the shock profile is uniform on either side of the subshock; this limit corresponds to the first run in the iteration sequence described in §§ 3.2 and 3.3 and has been studied in detail in Ellison et al. (1995). Several interacting elements of the code, including shock (or grid zone) crossings and the probability of return calculation (which includes the fluxweighting of momenta of the returning particles: see § A3 in the Appendix), must be implemented properly in order to yield the well-known test particle acceleration power law. The Fermi power law is achieved when particle speeds v far exceed the HT flow speed $u_{x1}/\cos \Theta_{Bn1}$. From analytic calculations (see, e.g., Drury 1983; Jones & Ellison 1991), the spectral index σ of the power law then depends only on the compression ratio $r = u_1/u_{2x}$ regardless of the obliquity or other plasma parameters. The compression ratio is determined from equations (4)–(9) with $\dot{Q}_{esc} = P_{xz} = 0$ (see also Decker 1988). For nonrelativistic particle energies and shock speeds, the test particle distribution is

$$\frac{dJ}{dE} \propto E^{-\sigma}, \quad \sigma = \frac{r+2}{2(r-1)}, \quad (18)$$

where dJ/dE is the number of particles in units of (cm² s sr eV)⁻¹, i.e., is an omnidirectional flux (see Jones & Ellison 1991). The reproducibility of this form is a powerful tool for debugging the portions of the code that are directly related to the transport and acceleration of particles. It is instructive to review test article distributions before proceeding to our results for the nonlinear problem.

In Figure 2 we show spectra calculated with a discontinuous shock for three different sets of parameters and for both large-angle scattering (*solid lines*) and pitch-angle diffusion (*dotted lines*). Note that the examples labeled (*c*) are multiplied by 0.01 for clarity of display. All spectra here and elsewhere are omnidirectional, are calculated several λ_0 (i.e.,



FIG. 2.—Test particle omnidirectional, distribution functions measured several λ_0 downstream from a discontinuous shock in the normal incidence frame. All spectra here and elsewhere are normalized to one particle per square centimeter per second injected far upstream. Each pair of histograms has obliquity, Mach numbers and η as indicated according to the labels (a), (b), and (c). The solid lines are results using large-angle scattering, while the dotted lines are for pitch-angle diffusion. At energies where $v \gg u_{x1}/\cos \Theta_{Bn1}$ applies, all spectra attain the canonical Fermi power law (solid lines of arbitrary normalization). Note that the spectra labeled (c) are multiplied by 0.01 for clarity. The similarities for the two modes of scattering are striking in these strong cross-field diffusion examples.

"thermal" mean free paths) downstream from the shock in the normal incidence frame, and are normalized to one particle per square centimeter per second injected far upstream. In all cases we have used $u_1 = 500$ km s⁻¹ and $n_1 = 1$ cm⁻³; the (sonic and Alfvénic) Mach number 20 cases here use $B_1 = 1.15 \times 10^{-5}$ G and $T_1 = 4.54 \times 10^4$ K, while the Mach number 3 case uses $B_1 = 7.64 \times 10^{-5}$ G and $T_1 = 2.02 \times 10^4$ K. The other parameters are given in the figure. No free escape boundary is included in these test article cases, since it is necessary only for the nonlinear acceleration problem.

Note that the compression ratio varies slightly between the two high Mach number examples, being r = 3.96 for the $\Theta_{Bn1} = 30^{\circ}$ case and r = 3.94 for the 60° case; this occurs because of a slight dependence of r on obliquity for noninfinite Mach numbers. For the low Mach number example (c), the shock is quite weak with r = 2.5. The Fermi power laws obtained from equation (18) for these compression ratios are shown as light solid lines in the figure (with adjusted normalization to aid visual distinction). Clearly the most important feature of Figure 2 is that the simulation does reproduce the Fermi power-law index at high energies for a wide range of shock parameters. Comparison of examples (a) and (b) with similar compression ratios but quite different Θ_{Bn1} supports the fact that the Fermi spectral index σ is determined solely by r.

The next most striking feature of these plots is that the two modes of scattering produce very little difference in the spectra. This difference is largest for portions of the $\Theta_{Bn1} = 60^{\circ}$ spectrum (b) between thermal energies and about 100 keV. There the distribution for the LAS mode (the solid line

in [b]) is somewhat noisy because of comparatively poor statistics in high- η , high-obliquity runs (i.e., weak injection: see Ellison et al. 1995), and this noise may obscure some underlying structure that can arise from large energy boosts in individual shock crossings. At these energies, the particle speed does not far exceed the HT frame flow speed u_{x1}/\cos Θ_{Bn1} , which leads to significant anisotropies in the particle population and, more importantly, to measurable differences in the degree of anisotropy produced in PAD and LAS modes. Since such differences in angular distributions are responsible for observed differences between LAS and PAD applications to unmodified relativistic shocks (e.g., see Ellison et al. 1990a for a comparison of the modes and Kirk & Schneider 1987 and Ostrowski 1991 for PAD cases), it is not surprising that spectral differences should appear here at suprathermal energies for highly oblique shocks. Clearly, Figure 2 shows that for this intermediate-obliquity case, the mode of scattering has virtually no effect on the resultant spectrum at either thermal or the highest energies and therefore that the scattering mode plays little role here in determining the efficiency of acceleration, i.e., the fractional energy deposited in high-energy particles. This is not surprising, because of the low value of η here: we naturally expect that strong scattering (near the Bohm diffusion limit) will destroy any sensitivity of the acceleration process to the shock obliquity or distribution anisotropies and hence the type of scattering. In very weak scattering (large η), large differences between the scattering modes may occur even for low obliquities.

Also evident in Figure 2 is the strong effect the input parameters have on injection efficiency: the $\Theta_{Bn} = 60^{\circ}$ spectra fall an order of magnitude below the $\Theta_{Bn} = 30^{\circ}$ spectra at high energies even though they both obtain the same power-law index. Increasing either Θ_{Bn1} or η will result in decreased injection efficiency. These effects were detailed in Ellison et al. (1995), where an anticorrelation between acceleration time and efficiency of acceleration in test article shocks was observed. We note that existing analytic predictions for the transition between the thermal peak and the high-energy power law, i.e., the injection efficiency, require ad hoc parameters additional to and independent of those made for the shock structure to connect the thermal gas to the cosmic-ray population (see, e.g., Zank, Webb, & Donohue 1993; Kang & Jones 1995; Malkov & Völk 1995). The advantage of our model is that the single relation (eq. [1]) controls the shock structure, the absolute injection efficiency, and, in fact, the entire shock solution. This makes it straightforward to compare model predictions to observations and to infer plasma properties (such as the level of turbulence, the correctness of the elastic scattering assumption, etc.) from these comparisons, an attractive feature. Properties of upstream particle distributions are deferred to the discussion of nonlinear results in the next subsection, though test particle spectra upstream of oblique shocks were presented in Baring, Ellison, & Jones (1994).

The difference in statistics seen in Figure 2, i.e., LAS spectra are noisier than PAD spectra, comes about because changes in particle pitch angles, phases, and energies are more frequent in the PAD case than for LAS, i.e., many small pitch-angle changes versus a single isotropizing event. Consequently, the acceleration process is more continuous with PAD, and the spectra produced are smoother than for LAS, where discreteness in the scattering can sometimes

introduce spectral structure due to reflection (see, e.g., Baring et al. 1994). When scattering is strong, these two modes give very similar statistics, but in weak scattering, large differences can occur, particularly for large obliquities, when poorer statistics inhibit the quality of the LAS spectra.

4.2. Examples Showing Iteration of Shock Profile

For our next examples, we compute the self-consistent smooth shock profile beginning with a low Mach number case, i.e., $M_{A1} = M_{S1} = 3$, $\Theta_{Bn1} = 30^{\circ}$, $d_{FEB} = -50\lambda_0$, and $\eta = 2$, yielding a plasma β of $\beta_1 = 1.2$. This corresponds to a weak shock, typical of interplanetary shocks observed in the heliosphere (e.g., see Burton et al. 1992; Baring et al. 1995b). To reiterate, in the results that follow, all lengths are measured in units of λ_0 , which is the mean free path ηr_{g1} of a proton of gyroradius $r_{g1} = m_p u_1 c/(eB_1)$, i.e., with the speed u_1 in the upstream magnetic field.

In the left-hand panels of Figure 3, we depict the average flow speed, u_x , the flux $F'_{xx}(x)$ of the x-component of momentum, and the energy flux $F'_{en}(x)$, all normalized to far upstream values, for several iterations starting from a discontinuous shock (*light solid line*) and yielding the final profile (*heavy solid line*). These iterations were done using LAS and an overall compression ratio of $r \simeq 2.7$ that was determined in previous iterations on r. The Rankine-Hugoniot compression ratio with $Q_{esc} = 0$ is r = 2.67, which is equal (within errors) to our 2.7 value. The convergence is quite rapid, and the heavy solid lines (fourth iteration) show no further statistically significant change with additional iterations. Except for a departure of about 5% near x = 0, the flux of the x-component of momentum (middle panels) is constant for all x after the final shock profile has been obtained. The flux F'_{xz1} of the z-component of momentum is generally small and less interesting; its profile (and those of u_z and B_z) is not displayed for reasons of brevity. For the discontinuous shock (light solid lines), the momentum flux was clearly not conserved and rose to $\sim 140\%$ of the far upstream value downstream from the shock.

The escaping energy flux at the FEB (which is at $-50\lambda_0$ and is not shown in the figure) is less than 1% of the far upstream value and does not influence the overall compression ratio significantly. The check on the consistency of the final profile is that the momentum flux and the energy flux, including the escaping flux, must both be conserved. When this is achieved (i.e., corresponding to the solid lines), we



FIG. 3.—Flow and flux profiles for quantities in the x-direction for a weak shock with parameters $M_{A1} = 3$, $M_{S1} = 3$, $\Theta_{Bn1} = 30^\circ$, $d_{FEB} = -50\lambda_0$, $\eta = 2$, and a self-consistently determined compression ratio, r = 2.7. The three left-hand panels show the x-component of the flow speed, the flux $F'_{xx}(x)$ of the x-component of momentum, and the energy flux for large-angle scattering. All quantities are measured in units of the far upstream values (UpS). The three right-hand panels show the same quantities for pitch-angle diffusion. In all cases, four iterations are shown; the first with a light solid line, the second with a dashed line, the third with a dot-dashed line, and the fourth with a heavy solid line (the flat dotted line indicates upstream values). After four iterations, all quantities remain the same except for statistical variations. The momentum and energy fluxes are conserved everywhere to within 10%. Note that previous iterations (not shown) were done to determine the compression ratio. The different scattering modes produce identical results within statistics.

have a unique, self-consistent solution. The $\sim 10\%$ discrepancy in the energy flux near x = 0 is most likely the result of the strong gradients in the shock and/or agyrotropic pressure tensor terms in the Rankine-Hugoniot relations, which we have neglected from our flux considerations. This discrepancy decreases rapidly with increasing Mach number and so is greatest for this present case.

Figure 3 also shows the shock structure obtained with pitch-angle diffusion PAD (*right-hand panels*), all other shock parameters being the same as the LAS case. Within statistics, the two scattering modes give identical results, both for the shape of the profile and the overall compression ratio. This feature is not surprising, given that the test particle results of the previous simulation bore this similarity out.

In Figure 4, we show the distribution functions generated by the smooth shocks of Figure 3. The spectra are omnidirectional, measured downstream from the shock, and calculated in the shock (i.e., NIF) frame. As with the shock structure, the distribution functions obtained with the two scattering modes are identical within statistics. This is to be expected because $\eta = 2$ is close to the Bohm diffusion limit where, as mentioned above, isotropic diffusion will naturally obscure the differences between PAD and LAS. There is a large difference, however, between the smooth shock results and the test particle, discontinuous shock (dotted *line*), which was obtained using the same compression ratio (r = 2.7) computed in the self-consistent solution of the nonlinear LAS simulation. The light solid line is the Fermi power law expected from r = 2.7; the test particle spectrum attains this result before the falloff at ~ 100 keV produced by the FEB. The discontinuous shock produces more efficient acceleration at low energies than the smooth shock,



FIG. 4.—Distribution functions measured downstream from the shock in the shock (or normal incident) frame obtained from the profiles shown in Fig. 3. The turnover at $E \sim 200$ keV is the result of particles leaving at the upstream FEB. Apart from statistics, there are no discernible differences between the large-angle scattering and pitch-angle diffusion scattering modes. For comparison, the dotted line shows the test particle spectrum obtained for the same shock parameters, and the light solid line is the expected Fermi power law (arbitrary normalization) for r = 2.7.

which follows from the nature of the smoothed shock profile: low-energy particles feel the effect of the subshock, whereas only the high-energy particles sample the full compression ratio of r = 2.7. This same property is responsible for the upward curvature of the nonlinear spectra, which never attain the Fermi power law, but flatten toward it before falling off because of the FEB.

We have also obtained solutions (not shown) using exactly the same parameters as above except with a FEB at $d_{\text{FEB}} = -10\lambda_0$. The smaller shock system causes a cutoff at a lower energy than seen in Figure 4, and the shock structure is correspondingly on smaller length scales. However, the self-consistent compression ratio is still $r \sim 2.7$, consistent with a $Q_{\text{esc}} = 0$, as expected, since these low Mach number shocks put a small fraction of the available energy into energetic particles regardless of the shock size.

As a more extreme example, we show in Figure 5 a high Mach number shock ($M_{S1} = M_{A1} = 20$) with a much larger shock size, i.e., the FEB is at $d_{\text{FEB}} = -200\lambda_0$. The other input parameters are $u_1 = 500$ km s⁻¹, $n_1 = 1$ cm⁻³, $\Theta_{Bn1} = 30^\circ$, $\eta = 2$, $B_1 = 1.15 \times 10^{-5}$ G, and $T_1 = 4.54 \times 10^4$ K, yielding $\beta = 1.2$. We show only the LAS scattering mode since the PAD results are essentially identical. Note that the self-consistent compression ratio used here is r = 5.2 (well above the R-H value of r = 3.96), which has been determined with previous runs not shown. The distance scale in Figure 5 is logarithmic for $x < -10\lambda_0$ and linear for $x > -10\lambda_0$.

There are several important features of this shock solution. In the first iteration with no shock smoothing, the momentum and energy fluxes are wildly nonconserved with both of them obtaining downstream fluxes almost 15 times as large as the upstream values. Despite this, the subsequent iterations converge rapidly, and by the fourth iteration, the momentum flux is conserved everywhere to within 5% of the upstream value (the first, second, third, and fourth iterations are shown by light solid, dashed, dashed-dot, and heavy solid lines, respectively; the flat dotted line indicates the far upstream value). The effects from the anisotropic terms in the momentum and energy fluxes are less noticeable here than in the previous low Mach number examples. As with the previous examples, the shock is smoothed out to the FEB; however, the subshock here is considerably more distinct, showing a sharp discontinuity between the flow just upstream from the subshock and the downstream flow. The width of the subshock is well within $1\lambda_0$.

As for the energy flux, it falls about 20% below the far upstream value because of the particles lost at the FEB. The escaping energy flux, Q_{esc} , which is zero far upstream, falls rapidly around d_{FEB} and then becomes approximately constant into the downstream region. This results in a compression ratio, obtained by iteration in previous runs, of $r \simeq 5.2$, compared to the R-H value of r = 3.96. A compression ratio of r = 5.2 implies $Q'_{esc} = 0.098$ and a $Q'_{esc}/F'_{en1} \simeq 0.19$, and when this is added to the energy flux shown in the bottom panel of Figure 5, we have a self-consistent solution with all fluxes constant at all x to within a few percent. Larger escaping fluxes are expected for such high Mach number shocks because their greater compression ratios enhance the acceleration efficiency to the highest energies.

The complete shock structure is shown in Figure 6, where we have included along with $u_x(x)$, the z-component of flow speed, $u_z(x)$, the angle the local magnetic field makes with the shock normal, $\Theta_{Bn}(x)$, and the total magnetic field mag-



FIG. 5.—The top panel shows the x-component of flow speed vs. x. The next two panels show the flux $F'_{xx}(x)$ of the x-component of momentum, and the bottom two panels show the energy flux. The shock parameters are $M_{S1} = M_{A1} = 20$, $d_{FEB} = -200\lambda_0$, $u_1 = 500$ km s⁻¹, $n_1 = 1$ cm⁻³, $\Theta_{Bn1} = 30^\circ$, and $\eta = 2$. In all cases, four iterations are shown: the first, second, third, and fourth iterations are shown by light solid lines, dashed lines, dashed-dot lines, and heavy solid lines, respectively, and the horizontal scale is logarithmic for $x < -10\lambda_0$ and linear for $x > -10\lambda_0$. After four iterations, no further changes occur in the profiles, and momentum and energy are conserved across the shock once the escaping energy flux ($Q'_{esc}/F'_{en1} \simeq 0.19$) is accounted for. Note that previous iterations were performed to obtain the self-consistent compression ratio, $r \simeq 5.2$.

nitude, $B_{tot}(x)$. The solid lines show the final shock structure, and this is compared to the initial structure shown by dotted lines. As noted above, both the shape and the overall compression ratio must be modified to obtain a selfconsistent solution, and this translates to a change from the R-H values in the downstream u_{z2} , Θ_{Bn2} , and B_2 as indicated by the dotted lines. The sharpness of the subshock in Figure 6 at x = 0 is partially an artifact of how we smooth and truncate the flow profile between iterations. As mentioned above, we average the predicted profile with the previous one, and, since we start with a discontinuous shock, some sharpness persists. We also set all predicted values of u_x to u_{x2} at $x > 1\lambda_0$. Despite this, the subshock is, in fact, quite sharp as we discuss at the end of this section.

In Figure 7 we show (*solid line*) the downstream, shock frame distribution function obtained in the smooth shock solution just described. It differs considerably from the test



FIG. 6.—Complete shock structure (*solid lines*) for the example shown in Fig. 5, again with a composite distance scale. The dotted lines show the discontinuous shock structure with the initial R-H compression ratio, r = 3.96. The final shock has a overall compression ratio of $r \simeq 5.2$.

particle solution (dotted line) in that the downstream thermal peak is at a lower energy, the temperature is slightly lower, and far fewer thermal particles become accelerated. The straight line is the power-law slope expected from the test particle Fermi solution with r = 5.2 and matches our test particle solution at energies well above thermal and below where the FEB becomes important. The smooth shock solution, however, does not attain the test particle power law and remains considerably steeper. This can be understood by examining the top panel of Figure 5 where it can be seen that at $d_{\text{FEB}} = -200\lambda_0$, there is enough escaping energy flux to smooth the shock further upstream from this point. Particles leave the shock at the FEB before feeling the full compression ratio.

To complete this example, we show in Figure 8 distribution functions at various x-positions, i.e., $x = -50\lambda_0$ (dotted line), $x = -4\lambda_0$ (dashed line), $x = -0.5\lambda_0$ (light solid line), and $x = +\lambda_0$ (heavy solid line). At observation points far upstream from the shock, only the unshocked thermal peak is present since energetic particles from the shock are not able to diffuse against the background flow to reach the observation point. As the upstream observation point moves toward the shock, two things happen. First, the highest energy particles begin to show their presence, and second, the thermal peak from particles that have not yet crossed the shock begins to shift to lower energy (see insert where we have plotted the thermal peaks of the $x = -50\lambda_0$ and $x = -0.5\lambda_0$ spectra). Since we take $\lambda \propto r_q$, the diffusion length increases with energy, and higher energy particles from the shock are able to stream farther upstream than low-energy ones; thus, as the observation point moves toward the shock, the spectrum fills in from high energy to



FIG. 7.—The downstream, shock frame distribution functions for the smooth shock obtained in Fig. 5 (*heavy solid line*) and a test particle shock (*dotted line*) with the same parameters including a compression ratio of 5.2. Note the shift of the thermal peak to lower energy that occurs in the smooth shock. The light solid line shows the test particle, power-law slope expected from Fermi acceleration for a shock with r = 5.2. This is obtained by the discontinuous shock solution before the falloff produced by the FEB but not by the smooth shock solution.

low (this property was recognized, for test particle situations, by Baring et al. 1994). The shift in the thermal peak arises because spectra calculated in the shock frame shift to lower energy as the bulk flow speed falls as the shock is



FIG. 8.—Shock frame distribution functions calculated at $x = -50\lambda_0$ (dotted line), $x = -4\lambda_0$ (dashed line), $x = -0.5\lambda_0$ (light solid line), and $x = +\lambda_0$ (heavy solid line) for the smooth shock obtained in Fig. 5. The insert shows the thermal peaks for the $x = -50\lambda_0$ and $x = -0.5\lambda_0$ cases on a linear energy scale. The $-4\lambda_0$ thermal peak lies between these two.

approached. The slowing of the bulk flow in the shock precursor also heats the incoming particles somewhat before they encounter the sharp subshock lowering the local Mach number. These features are well-defined model predictions that can be tested against observations.

In Figure 9 we show the upstream scale height for particles of various energies. The ordinate is the ratio of the flux at x over the flux at x = 0 for a given energy. As expected, the length scale (i.e., the distance at which the flux *e*-folds) is largest for the highest energy particles, and the fluxes fall off exponentially with distance from the shock (a property of diffusion against the convecting flow). It is also important to note that low-energy particles (i.e., the 3 and 10 keV examples) can have extremely short upstream precursors. Particle detectors on spacecraft being overtaken by interplanetary shocks will see very different time profiles depending on the particle energy sampled and may, depending on the time integration of the spectrometer (which is usually long compared with typical gyroperiods), see a step function increase in intensity at low energies simultaneously with a slow rise in high energy particles. This effect may explain some puzzling aspects of recent Ulysses observations that have led to the suggestion that a two-stage acceleration mechanism operates for pickup protons (Gloeckler et al. 1994).

As our final example, we show in Figure 10 a highly oblique shock ($\Theta_{Bn1} = 75^{\circ}$) with $M_{S1} = M_{A1} = 10$, $d_{FEB} = -20\lambda_0$, $\eta = 5$ and using large-angle scattering. For these parameters, little acceleration occurs, and the shock profile is nearly discontinuous. Nevertheless, the little smoothing evident in the top panel of Figure 10 is enough to reduce the energy flux from being ~20% above the far upstream value to a constant value. Because of the inefficient acceleration, few particles, carrying very little energy flux, escape at the FEB, so there is no need to adjust the compression ratio. The final ratio is r = 3.74, effectively the R-H value. We have done the same calculation with the same parameters except using pitch-angle diffusion and find essentially the



FIG. 9.—Ratio of the omnidirectional flux, dJ/dE, at position x to the flux at x = 0 for a given energy vs. distance upstream from the shock shown in Fig. 5. These are determined from the spectra shown in Fig. 8 and define the scale heights for the several energies indicated on the figure.



FIG. 10.—The three panels show the x-component of the flow speed, the flux $F'_{xx}(x)$ of the x-component of momentum, and the energy flux for a shock with $\Theta_{Bn1} = 75^{\circ}$, $M_{S1} = M_{A1} = 10$, $d_{\text{FEB}} = -20\lambda_0$, $\eta = 5$, and large-angle scattering. The profile for the PAD case is essentially the same and is not shown. In all panels, the first, second, third, and fourth iterations are shown by light solid lines, dashed lines, dashed-dot lines, and heavy solid lines, respectively. Comparatively little acceleration takes place, and the final shock profile is very nearly discontinuous with the R-H compression ratio, r = 3.74.

same profile (which is not shown), although some slight differences do show up in the distribution functions.

The top two curves in Figure 11 are the distribution function from the LAS example (solid line) along with the distribution produced in a shock with the same parameters as that shown in Figure 10, only using PAD (dashed line). The main difference between the two cases is that the PAD distribution is somewhat smoother than the LAS one. The PAD shock is also somewhat less efficient in accelerating particles to the highest energies. In general, however, even at this large obliquity, the choice of scattering mode does not play a dominant role in determining the acceleration efficiency. The lower two curves (multiplied by 0.01 for clarity) are test particle results and are similar to the distribution functions produced by the smooth shock but are slightly flatter, as expected. No portions of these examples elicit the Fermi, test particle power-law slope (dotted line) but are clearly flattening toward it before the FEB causes the spectra to turn over.

Finally, we comment on the sharpness of the subshock seen in all of the examples we have presented. As mentioned above, part of this is due to the scheme we have for iterating the profile and insuring rapid convergence. We average the predicted profile with the previous one, make the predicted profile monotonic, and set all predicted values of $u_x(x)$ to u_{x2} for $x > \lambda_0$. In Figure 12, we show the same final $u_x(x)$ plots as shown in the top left-hand panel of Figure 3, the



FIG. 11.—Distribution functions for the highly oblique shock ($\Theta_{Bn1} = 75^\circ$) shown in Fig. 10. The top two curves are smooth shock solutions using LAS (*solid line*) and PAD (*dashed line*). The lower two curves are test particle results. The straight dotted line shows the slope expected from the standard Fermi power law. Unlike our examples at lower obliquities, clear differences exist depending on the type of scattering, although these are not great enough to produce noticeable differences in the shock profile.



FIG. 12.—Comparison of $u_x(x)/u_1$ predicted by the simulation (solid lines) with $\langle v_x \rangle$ (dotted lines) plotted with a linear distance scale. The top panel is the example shown in the top left-hand panel of Fig. 3, the middle panel is the shock shown in Fig. 5, and the bottom panel is the shock shown in Fig. 10. While some sharpness of the shock profile is the result of our smoothing procedures, the subshock transition is less than $1\lambda_0$ wide in all cases.

top panel of Figure 5, and the top panel of Figure 10, except here they are all plotted on an expanded linear distance scale (solid lines). The dotted lines in Figure 12 are the calcu*lated* $\langle v_x \rangle$ obtained from distributions produced by the simulation using the solid line shock profiles. In all cases, a clear subshock exists that is considerably less than λ_0 in width, and the mean velocities are nearly as sharp as our processed profiles except for statistical fluctuations and the truncation we impose at $x > \lambda_0$. Outside the range shown, u_x and $\langle v_x \rangle$ are indistinguishable except for noise. While comparing u_x and $\langle v_x \rangle$ is somewhat artificial since $\langle v_x \rangle$ is calculated using u_x , the small broadening of the flow speed around $x \sim 0$ does not have an appreciable influence on the momentum and energy fluxes. We have performed simulations using $\langle v_x \rangle$ instead of $u_x(x)$, and the momentum and energy fluxes remain within $\sim 10\%$ of the conserved values at all x. For our purposes, since we do not attempt to model scales less than a convected thermal ion gyroradius, there is essentially no difference between the $u_x(x)$ used in the simulation and $\langle v_x \rangle$.

4.3. Injection and Acceleration Efficiency

A quantity that is central to the acceleration problem is the efficiency of the Fermi mechanism. It can be defined in a variety of ways: we define the acceleration efficiency, $\epsilon(>E)$, at or behind the shock as the downstream energy flux above energy E divided by the incoming energy flux, i.e.,

$$\epsilon(>E) = \frac{\zeta P(>E)u_{x2} + Q_{\rm esc}(>E)}{\zeta P_1 u_1 + \rho_1 u_1^3 / 2 + B_{z1}^2 u_1 / (4\pi)}, \quad \zeta = \frac{\gamma}{\gamma - 1}, \quad (19)$$

where P(>E) is the downstream pressure and $Q_{esc}(>E)$ is the escaping energy flux, both in particles with energies greater than E. The pressure is obtained by taking 2/3 of the energy density in the omnidirectional distribution, dJ/dE.

In Figure 13 we show $\epsilon(>E)$ for our three previous nonlinear examples, i.e., curve (a) is for the LAS case shown in Figure 4, (b) is for the case shown in Figure 7, and (c) is for the LAS, smooth shock case shown in Figure 11. As is apparent from the figure, large differences in the efficiency depending on Θ_{Bn1} , the Mach number, η , and the distance to the FEB occur. Examples (b) and (c) both accelerate particles to above 1000 keV and have similar Mach numbers, but the highly oblique shock (c) is much less efficient. Examples (a) and (b) have the same $\Theta_{Bn1} = 30^{\circ}$ but differ considerably in Mach numbers (3 versus 20, respectively), with (b) being more efficient because its higher Mach number generates a larger compression ratio. At this stage of our work, there appears to be no simple way to characterize the injection and acceleration efficiency of oblique shocks, but the trends with obliquity and Mach number are quite clear. Note that the efficiency curves in Figure 13 have been normalized to $\epsilon(>0) = 1$ to facilitate comparison. The unnormalized curves differ by small amounts (<10%) from $\epsilon(>0) = 1$ due to simulation statistics.

Another point that should be made concerning Figure 13 is that we choose to define our efficiency as a function of energy. If we do not have an independent source of energetic seed particles, all accelerated particles must originate as thermal particles, and they will be drawn more or less continuously from the thermal population—there will be no clear separation between thermal and energetic particles. Our identical treatment of the thermal and nonthermal populations is why we do not need to define an "injection



FIG. 13.—The acceleration efficiency, as defined in eq. (19) (i.e., the total energy flux in particles with energy above *E*), as a function of particle energy. The solid curve (*a*) is calculated from the LAS spectrum shown in Fig. 4, the dashed curve (*b*) is calculated from the smooth shock spectrum shown in Fig. 7, $M_{A1} = M_{S1} = 20$), and curve (*c*) is calculated from the LAS, smooth shock solution shown in Fig. 11.

energy." However, there are ways to prescribe efficiencies qualitatively that describe the overall distribution rather than different particle energies. For example, while all three cases in Figure 13 have comparable efficiency at around 0.8 keV, this energy does not define the approximate juncture between thermal and nonthermal populations for cases (a) and (c), whereas it does for case (b). This juncture is roughly represented by the upward kinks at energies 3 and 1.7 keV for cases (a) and (c), respectively. Hence, the ratio of downstream nonthermal to thermal energy densities for the three cases are roughly (a) 0.2, (b) 0.5, and (c) 0.15; these numbers could be taken as an alternative measure of acceleration efficiency.

5. DISCUSSION AND CONCLUSIONS

A host of observational evidence, both direct and indirect, confirms that collisionless shocks in space accelerate particles with high efficiency. Possibly a large fraction of all nonthermal particle populations in diffuse regions of space are generated by shocks, which makes shock acceleration one of the most important problems in high-energy astrophysics. As a step toward a full understanding of shock acceleration, we have developed a model that combines nonlinear particle acceleration and diffusion with shock dissipation and nonlinear hydrodynamics forming the shock structure. This paper presents both the details of our simulation technique and representative acceleration results as a prelude to a more comprehensive survey of the parameter space associated with modified, oblique shocks. While our model is still incomplete, with simplifying assumptions concerning the microphysical processes involved, we believe it is the most realistic current solution of the steady state shock acceleration problem. We include (1) a strongly energy-dependent diffusion coefficient (see eq. [1]), which models cross-field diffusion; (2) the ability to model either

large-angle scattering or pitch-angle diffusion; (3) injection from the thermal background with no additional free parameters; (4) the determination of the self-consistent, average shock structure including the dynamic effects of accelerated particles on the thermal shock; (5) the dynamic effects of particle escape from finite shocks; and (6) shock drift and compressional acceleration simultaneously. Principal results of this paper include downstream spectra (see Figs. 4, 7, and 11), properties of upstream populations (see Figs. 8 and 9), and acceleration efficiencies (Fig. 13). The Monte Carlo simulation does not treat (1) a self-consistent determination of the diffusion coefficient from wave-particle interactions, (2) time-dependent effects, (3) relativistic particles or flow speeds, (4) a cross-shock potential due to charge separation, or (5) geometry other than a plane shock.

Clearly the most important omission is the self-consistent determination of the diffusion coefficient. Our results hinge on the energy-dependent form we have assumed for κ , which is motivated by previous theoretical analyses (see Jokipii 1987; Giacalone et al. 1992; Ellison et al. 1995), and also observational constraints at parallel shocks (see Ellison et al. 1990b; Ellison & Reynolds 1991). However, the selfconsistent determination of κ requires knowledge of the microphysics, and only plasma simulations where the electric and magnetic fields are calculated directly from particle motions (see, e.g., Quest 1988) can give this information. These simulations are extremely demanding computationally and will not, in the foreseeable future, be able to model particle acceleration in shocks adequately to astrophysically important energies. The recent work of Jokipii et al. (Jokipii et al. 1993; Giacalone, Jokipii, & Kóta 1994; Jokipii & Jones 1996) has shown that if a coordinate is ignorable (as in one- or two-dimensional hybrid simulations), cross-field diffusion effects are suppressed, and since cross-field diffusion is an essential part of injection and acceleration in shocks (certainly oblique ones), threedimensional simulations must be used to model shocks. No existing computer is capable of running realistic threedimensional plasma simulations over dynamical ranges of energies appropriate to astrophysical applications (see, however, Hellinger, Mangeney, & Matthews 1996).

We emphasize that even though we model plane shocks and our scattering operator is a gross simplification of the complex plasma processes taking place in shocks, the operator is fully three-dimensional, includes cross-field diffusion, and may well produce more realistic results than current one- or two-dimensional plasma simulations. In fact, comparisons between our model and spacecraft observations of highly oblique interplanetary shocks (IPSs) (Baring et al. 1995b, 1996) suggest that this is the case. The spacecraft observations clearly show that highly oblique shocks inject and accelerate thermal particles, a result we can model accurately (see, e.g., Figs. 11 and 13), but one that, to our knowledge, all existing one- and two-dimensional plasma simulations fail to show (see, e.g., Liewer, Goldstein, & Omidi 1993; Liewer, Rath, & Goldstein 1995; Kucharek & Scholer 1995).

Virtually all analytic models of nonlinear shock acceleration have been restricted to parallel shocks; however, Jones & Kang (1995) have recently extended the cosmic-ray diffusion-advection equation approach to oblique geometry and have produced impressive fits to the *Ulysses* observations mentioned above (see, e.g., Baring et al. 1995b). However, all models based on the diffusion approximation (i.e., the requirement that particle speeds be large compared to flow speeds) are limited in their ability to treat thermal particles and must use additional free parameters to model injection. For example, the parallel shock model of Berezhko et al. (i.e., Berezhko, Yelshin, & Ksenofontov 1994; Berezhko, Ksenofontov, & Yelshin 1995b; Berezhko et al. 1995a) uses a source term for monoenergetic injection at the gas subshock that is treated as a discontinuity. Here, a small fraction ϵ of incoming gas is transferred to cosmic rays, the injected particles instantly obtaining a superthermal momentum, p_{inj} . Both ϵ and p_{inj} are free parameters, and the final results depend strongly on them. Moreover, for simplicity, p_{inj} is usually kept fixed, while other parameters such as η vary (e.g., see Kang & Jones 1996), thereby avoiding a description of the strong dependence p_{inj} has on some of these parameters (η is a specific example). The main advantage of our model is that the Monte Carlo description is not restricted to superthermal particles, and injection is treated self-consistently. Once a scattering description such as equation (1) is chosen, both the injection rate and the effective injection momentum are fully determined, as is the complete shock structure, by the Monte Carlo solution without any additional parameters such as ϵ . In fact, there is no "injection momentum" in our solution since particles are drawn smoothly from the background thermal gas.

The parameters that determine the injection and acceleration efficiency of shocks are the obliquity, Θ_{Bn1} , the strength of cross-field diffusion, η , the Mach numbers, M_{S1} and M_{A1} , and the size of the shock system (i.e., $|d_{\text{FEB}}|$). These all influence the shock in complex ways, and there is no simple relationship between them. In general, we can state that the acceleration efficiency (i.e., the fraction of energy flux that ends up in high-energy particles) increases with (1) decreasing Θ_{Bn1} , (2) decreasing η (i.e., stronger scattering), (3) increasing Mach number, and (4) increasing shock size. We have found that the differences in the shock structure and acceleration efficiency resulting from using either large-angle scattering (LAS) or pitch-angle diffusion (PAD) are generally small (e.g., see Fig. 2 for the test particle regime and Figs. 4 and 11 for full nonlinear results) for the parameter regime we have investigated, namely strong scattering and $v_{\rm HT} \ll c$, and can be neglected in the Bohm diffusion limit. However, the differences between the nonlinear results and the test particle ones are very large (see, e.g., Fig. 7) except for high obliquities (i.e., Fig. 11) or very low Mach numbers (Fig. 4), where the acceleration efficiency is low enough for the thermal gas to dominate the nonthermal population dynamically, and the shock profiles are very sharp.

For the first time, we have been able to calculate the absolute injection and acceleration efficiency of nonlinear oblique shocks without the use of an ad hoc injection parameter. Our results (Fig. 13) show how large differences in efficiency can occur as parameters change; however, we have not yet explored the vast parameter regime oblique geometry opens up. Our next step toward a more complete solution of the shock acceleration problem will be a survey intended to quantify the differences the various parameters make in the distribution function and overall efficiency. This will include determining the effect of varying equation (1) and will yield predictions for future spacecraft and plasma simulation results. The only way to constrain our η parameter is by comparing our results with direct observ-

ations of shocks or with three-dimensional plasma simulations. Since, to our knowledge, no three-dimensional simulation results showing significant acceleration exist, we will concentrate on spacecraft observations as they become available. As already mentioned, this work has begun with spectral comparisons to *Ulysses* observations of nearby interplanetary shocks (i.e., those not expected to encounter pick-up ions), and our preliminary comparisons with data from *Ulysses* have already indicated that strong scattering accompanies highly oblique IPSs, constraining η to values smaller than about 10 (Baring et al. 1995b, 1996). Our simulation produces particle distributions at different distances upstream and downstream of the subshock, thereby providing a wealth of model predictions for testing against observations.

Once we are successful in constraining our parameters with heliospheric shock observations, the next step will be to apply our results to shocks with no in situ particle observations, such as the termination shock and supernova remnant blast waves. This is another useful aspect of our model, and we expect to be able to make predictions for the relative injection and acceleration efficiency as a function of ionic composition for both thermal and pickup ions at the termination shock and to calculate how efficiency varies around the rim of a supernova remnant shock. Since relativistic particles are produced in these shocks, our model will soon be generalized to include relativistic particle energies.

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APPENDIX

This Appendix describes four technical aspects of the Monte Carlo simulation, namely (1) our description of pitch-angle diffusion, (2) how particles cross the shock and grid points (actually planes of discontinuity of the flow and field profiles) in the simulation, (3) the details of how the probability of particle return from beyond the downstream simulation "boundary" is determined, and (4) how we derive the form of the conservation of energy flux in equation (9).

A1. PITCH-ANGLE DIFFUSION

To summarize our implementation of pitch-angle diffusion (PAD), which has been given in detail in Ellison et al. (1990a), we simulate small-angle scattering effects by allowing the tip of the particle's fluid frame momentum vector p to undergo a random walk on the surface of a sphere. If the particle originally had a pitch angle, $\theta_B^0 = \arccos \{p \cdot B/|p| | B|\}$, and after a time δt undergoes a small change in direction of magnitude $\delta \theta$, its new pitch angle, θ_B^0 is related to the old by

$$\cos \theta_B^N = \cos \theta_B^O \cos \delta \theta - \sin \theta_B^O \sin \delta \theta \cos \phi , \qquad (A1)$$

where ϕ is the azimuthal angle of the momentum change δp measured relative to the plane defined by the original momentum p and B. After each scattering, a new phase angle around the magnetic field, ϕ_B^N , is determined from the old phase angle, ϕ_B^O , by

$$\phi_B^N = \phi_B^O + \arcsin\left[\frac{\sin\phi\sin\delta\theta}{\sin\theta_B^N}\right].$$
 (A2)

 $\delta\theta$ is randomly chosen from a uniform distribution between 0 and $\delta\theta_{max}$, and ϕ is randomly chosen from a uniform distribution between $-\pi$ and π , so that the tip of the momentum vector walks randomly over the surface of a sphere of radius p = |p|.

If the time required to accumulate deflections of the order of 90° is identified with the collision time, t_c , using a diffusion analysis, the relation between $\delta\theta_{max}$ and the mean free path λ was shown by Ellison et al. (1990a) to be

$$\delta\theta_{\rm max} = \sqrt{6 \, \frac{\delta t}{t_c}}\,,\tag{A3}$$

where $t_c = \lambda/v$. Pitch-angle diffusion is then defined by the regime $\delta t \ll t_c$. Clearly, using this approach implies a magnetic fluctuation correlation length smaller than the particle gyroradius; this method then becomes an approximation that is nevertheless still very convenient for implementation in Monte Carlo simulations. Note that in the limit of $\delta \theta_{\text{max}} \rightarrow \pi$, this prescription of PAD becomes equivalent to our scheme for large-angle scattering (see Ellison et al. 1990a).

Equations (A1) and (A2) then can be used to determine the coordinates of the new gyrocenter:

$$\begin{aligned} x_{\rm gc} &= x - r_g \, \cos \, \theta_B^N \, \cos \left(\phi_B^N - \frac{\pi}{2} \right) \sin \, \Theta_{Bn} \,, \\ y_{\rm gc} &= y + r_g \, \sin \, \theta_B^N \, \sin \left(\phi_B^N - \frac{\pi}{2} \right), \\ z_{\rm gc} &= z + r_g \, \sin \, \theta_B^N \, \cos \left(\phi_B^N - \frac{\pi}{2} \right) \cos \, \Theta_{Bn} \,, \end{aligned}$$
(A4)

where (x, y, z) is the position of the particle when it scatters. The phase offset of $\pi/2$ represents the differences between position and momentum vector phases. The gyroradius r_a remains unchanged in the PAD event (true also for large-angle scattering) since |B| is fixed at the point of scattering, and our assumption of elastic scattering leaves the magnitude of the momentum unchanged in the fluid frame. However, in contrast to the LAS case in which the particle's momentum vector is only updated after t_c on average, the momentum vector is updated after every δt for PAD.

A2. SHOCK OR GRID ZONE BOUNDARY CROSSING

When a particle crosses a grid zone boundary (there is no distinction in our code between the shock and any other grid boundary), its orbit is changed because the magnetic field changes direction and magnitude. The new values of the particle's pitch angle and phase are obtained from the assumption that the momentum in the HT frame remains unchanged at the zone boundary; this follows from the absence of drift electric fields in this frame. This method does not require that the magnetic moment be conserved; differences between gyrohelix computations at a flow interface and the adiabatic approximation are discussed by Terasawa (1979).

The detailed calculation (see also Decker 1988; Begelman & Kirk 1990; Ostrowski 1991; and Takahara & Terasawa 1991) is as follows (the geometry is illustrated in Fig. 14). The component of the old momentum (i.e., the momentum before crossing the grid zone boundary) in the y-direction is given by

$$p_{y} = p_{\perp}^{O} \sin \phi_{B}^{O} , \qquad (A5)$$

and the component along the z'-direction is

$$p_{z'} = p_{\perp}^O \cos \phi_B^O \,, \tag{A6}$$

 $\Theta_{\!Bn,i+1}$

Х

B_{i+1}

 $\Delta \Theta_{Bn}$

0 р_В

where p_{i}^{O} is the component of momentum perpendicular to B_{i} , and z' is perpendicular to the y- B_{i} plane. Note that all momenta in this section are measured in the HT frame. The component of momentum along the z''-direction (i.e., the axis perpendicular

р⁰

1

Ζ

ΔE

Z''

Θ Bn.i



FIG. 14.—The geometry for calculating the gyroradius and phase of particles crossing a grid zone boundary. The boundary occurs at the kink in B.

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to the y- B_{i+1} plane) is given by

$$p_{z''} = p_{z'} \cos \Delta \Theta_{Bn} - p_B^O \sin \Delta \Theta_{Bn} , \qquad (A7)$$

where $\Delta \Theta_{Bn}$ is the difference in Θ_{Bn} across the grid zone boundary. The total momentum perpendicular to the new magnetic field direction, B_{i+1} , is

$$p_{\perp}^{N} = \sqrt{p_{y}^{2} + p_{z''}^{2}} , \qquad (A8)$$

and the new momentum parallel to the new magnetic field direction is

$$p_B^N = p_B^O \cos \Delta \Theta_{Bn} + p_{z'} \sin \Delta \Theta_{Bn} .$$
(A9)

Finally, the new phase around B_{i+1} is given by

$$\phi_B^N = \arctan \frac{p_y}{p_{z''}} \,. \tag{A10}$$

A3. THE PROBABILITY OF RETURN CALCULATION

The details of how particle return from the far side of the downstream return boundary (DRB) is effected are presented here; such return boundaries are found not only in our Monte Carlo technique but also in hybrid plasma simulations (see, e.g., Bennett & Ellison 1995). Assume a uniform flow with a component of velocity in the positive x-direction of u_{x2} and assume that particles in the local fluid frame are isotropic and of speed v_F . Quantities denoted by subscript F are measured in this fluid (plasma) frame.

The flux of particles crossing a y-z plane that is parallel to, and downstream of, the subshock interface is proportional to v_{xsk} , the x-component of particle speed in any frame in which the shock is at rest. Here $v_{xsk} > 0$ (<0) for transmissions to the downstream (upstream) side of the DRB. The probability that particles return to the DRB after crossing it from the upstream side is therefore simply (e.g., see Jones & Ellison 1991) the ratio of the flux of particles moving upstream of the DRB to the flux of particles moving to the downstream side of this plane. Clearly $0 < v_{xsk} < v_F + u_{x2}$ defines downstream crossings of the DRB, while $-v_F + u_{x2} < v_{xsk} < 0$ prescribes upstream crossings. We confine the discussion to cases with $v_F \ge u_{x2}$. Integrating over the angle of the particle velocity relative to the shock normal, or alternatively over v_{xsk} , the probability of return P_{ret} to the DRB for isotropic particles of speed v_F is

$$P_{\rm ret} = \left| \frac{\int_{-v_F + u_{x2}}^{0} v_{xsk} \, dv_{xsk}}{\int_{0}^{v_F + u_{x2}} v_{xsk} \, dv_{xsk}} \right| = \left(\frac{v_F - u_{x2}}{v_F + u_{x2}} \right)^2 \,. \tag{A11}$$

This expression is valid for any shock obliquity and is relativistically correct (Peacock 1981). It applies to all $v_F \ge u_{x2}$ (for $v_F < u_{x2}$, $P_{ret} = 0$), and the only requirements for its validity are that the particles be isotropic in the local fluid frame and that they do not change speed in the region to the right of the return plane. To ensure isotropy, we apply equation (A11) only after particles have scattered at least once in the downstream region when LAS is used or that particles have diffused through 90° in the downstream region when PAD is used. The decision for return, or otherwise, is made via a random number generator.

Now, consider only those particles that return back across the return plane. Both their pitch angle relative to the magnetic field, $\theta_B = \arccos \{ p \cdot B / |p| | B| \}$, and their phase around the magnetic field, ϕ_B must be determined in the fluid frame. Determining these requires knowledge of v_{xsk} for the returning particles, which can be computed by again noting that the flux of particles returning across the return plane (moving in the negative x-direction) is proportional to v_{xsk} . This means that the number of particles returning with v_{xsk} between v_{xsk} and $v_{xsk} + dv_{xsk}$ is proportional to $v_{xsk} dv_{xsk}$. So, for a particular v_F , returning particles are drawn from a distribution such that

$$\frac{2}{(v_F - u_{x2})^2} \int_0^{-|v_{xsk}|} v'_{xsk} \, dv'_{xsk} = \int_0^{N_R} dN_R = N_R \,, \tag{A12}$$

where N_R is a random number uniformly distributed between 0 and 1, and the normalization factor is chosen so the integral between 0 and $-v_F + u_{x2}$ equals one. Therefore,

$$v_{xsk} = \sqrt{N_R}(-v_F + u_{x2}),$$
 (A13)

and from this the x-component of speed in the plasma frame

$$v_{xF} = v_{xsk} - u_{x2} = -v_F \sqrt{N_R} - u_{x2}(1 - \sqrt{N_R})$$
(A14)

can be obtained. Choosing a series of random numbers, N_R , between 0 and 1 gives the proper distribution of returning particles.

To determine θ_B and ϕ_B in the fluid frame, we assume that particles will return distributed symmetrically around the x-axis in the fluid frame, a consequence of isotropy. This symmetry appears also in a shock frame (see Fig. 15), where the flow is orthogonal to the DRB, since phases are preserved in velocity transformations orthogonal to this plane. The velocity vector of a returning particle will make an angle θ_x in the fluid frame with the x-axis, given by $\cos \theta_x = v_{xF}/v_F = (v_{xsk} - u_{x2})/v_F$. If it also has an azimuthal angle about the x-axis of φ_x , chosen randomly between 0 and 2π , then from Figure 15, using spherical triangles, the values of the fluid frame pitch angle θ_B and phase ϕ_B can be expressed in terms of θ_x , φ_x , and



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FIG. 15.—The velocity vectors of returning particles (filled region in Fig. 15*a*) are symmetric about the *x*-axis. The vertical dashed line is at zero velocity in the shock frame, and the center of the v_F vectors is displaced by the flow speed, u_{x2} . Fig. 15*b* shows the spherical triangle, *abc*, used to calculate θ_B and ϕ_B . Points *a* and *b* lie in the *x*-*z* plane, while point *c* lies off the plane.

 Θ_{Bn2} , i.e.,

$$\cos \theta_{B} = \cos \Theta_{Bn2} \cos \theta_{x} + \sin \Theta_{Bn2} \sin \theta_{x} \cos (\pi - \varphi_{x}), \qquad (A15)$$

$$\cos \phi_B = \frac{\cos \theta_x - \cos \theta_B \cos \Theta_{Bn2}}{\sin \theta_B \sin \Theta_{Bn2}}.$$
 (A16)

Subsequently, the returning particle is placed at the downstream return plane and, using the new fluid frame phase and pitch angle (and also a new position for the guiding center), propagated upstream by transforming to the de Hoffmann–Teller frame. The statistical prescription in this subsection guarantees that our code effectively simulates an infinite region to the downstream side of the probability of return plane.

A4. THE ENERGY FLUX CONSERVATION EQUATION

While the pressure terms in the momentum fluxes in equations (7) and (8) are elementary to write down, derivation of the forms for the corresponding terms in the energy flux in equation (9) involve some subtleties. As outlined \S 3.1, we restrict the analysis to gyrotropic particle distributions in local fluid frames in the interest of simplicity; we believe that such an

In a local fluid frame somewhere in the shock environs, consider coordinate axes oriented so that the x-direction is aligned with the local magnetic field but such that a single rotation about the y-axis produces an identical orientation to the system depicted in Figure 1. In this coordinate system, a gyrotropic plasma has a diagonal pressure tensor, namely $P_{xx} \equiv P_{\parallel}$ and $P_{yy} = P_{zz} \equiv P_{\perp}$ with $P_{ij} = 0$ otherwise. P_{\parallel} and P_{\perp} are components of pressure parallel to and orthogonal to the ambient field and for a thermal plasma are related to analogous temperature components by two equations of state. Rotating the axes into alignment with the system in Figure 1 yields a nondiagonal pressure tensor \mathcal{P} due to mixing of the components:

$$\mathscr{P} = \mathscr{R} \begin{pmatrix} P_{\parallel} & 0 & 0\\ 0 & P_{\perp} & 0\\ 0 & 0 & P_{\perp} \end{pmatrix} \mathscr{R}^{-1}, \qquad \mathscr{R} = \begin{pmatrix} \cos \Theta_{Bn} & 0 & \sin \Theta_{Bn}\\ 0 & 1 & 0\\ -\sin \Theta_{Bn} & 0 & \cos \Theta_{Bn} \end{pmatrix},$$
(A17)

where \mathcal{R} is the rotation matrix. This gives a specific form for the pressure tensor of

$$\mathscr{P} = \begin{pmatrix} P_{\parallel} \cos^2 \Theta_{Bn} + P_{\perp} \sin^2 \Theta_{Bn} & 0 & (P_{\perp} - P_{\parallel}) \sin \Theta_{Bn} \cos \Theta_{Bn} \\ 0 & P_{\perp} & 0 \\ (P_{\perp} - P_{\parallel}) \sin \Theta_{Bn} \cos \Theta_{Bn} & 0 & P_{\parallel} \cos^2 \Theta_{Bn} + P_{\perp} \sin^2 \Theta_{Bn} \end{pmatrix}.$$
 (A18)

Since pressure represents the spread of velocities about the mean speed, the pressure tensor is invariant under bulk velocity transformations. Hence, it follows that equation (A18) defines the pressure in the normal incidence frame and therefore is directly applicable to the flux conservation considerations. The above coordinate rotation therefore yields the relationships

$$P_{\parallel} = P_{xx} + P_{xz} \tan \Theta_{Bn}$$

$$P_{\perp} = P_{xx} + P_{yz} \cot \Theta_{Bn},$$
(A19)

x

which define the components of the pressure tensor on the fluid frame in terms of normal incidence frame tensor components that can be simply determined using the structure of our simulation. At this point, it becomes apparent that the assumption of gyrotropy in the fluid frame is indeed expedient, since it enables complete specification of the fluid frame pressure tensor using only flux quantities measured in the NIF in the x-direction: generalizing from the gyrotropic approximation would require construction of coordinate grids in the other directions, thereby complicating the simulation immensely, with only marginal gain in physical accuracy.

The energy flux equation can now be simply constructed from the formalism in Boyd & Sanderson (1969, p. 56). The convective contribution to the energy flux is simply $P_{xx}u_x + P_{zz}u_z$. The thermal-type (i.e., velocity spread) term is usually written in the form $\rho k_B T u_x/(\gamma - 1)$ for temperature T, where k_B is Boltzmann's constant, and γ is the ratio of specific heats. For the nonthermal application here, prescribing the temperature is inappropriate, so we use an equation of state $\rho k_{\rm B}T =$ $\operatorname{Tr} \{\mathscr{P}\} = P_{\parallel} + 2P_{\perp}$ in order to generalize to nonthermal situations by converting to pressure formalism. It follows that

$$\frac{u_x}{B(\gamma - 1)} \left(P_{\parallel} + 2P_{\perp} \right) = \frac{u_x}{(\gamma - 1)} \left[P_{xx} + \frac{1}{3} P_{xz} (\tan \Theta_{Bn} + 2 \cot \Theta_{Bn}) \right]$$
(A20)

is the nonconvective contribution to the energy flux in the x-direction that results from particle pressure. This applies to both the nonrelativistic gases considered in this paper (with $\gamma = 5/3$) and also to more general cases with different equations of state (i.e., $4/3 < \gamma < 5/3$), including relativistic plasmas. Using the magnetic field identity $B_z/B_x = \tan \Theta_{Bn}$ then results in the form given in equation (9).

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