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Pitch-angle diffusion coefficients in test particle simulations and the estimation of the particle parallel mean free path

C Pleumreedaporn and A P Snodin

Department of Mathematics, Faculty of Applied Science, King Mongkut's University of Technology North Bangkok, Bangkok 10800, Thailand

E-mail: pim4599@hotmail.com

Abstract. The transport of energetic charged particles in turbulent magnetic fields is a topic of interest in various astrophysical contexts. In order to estimate the mean free path of a particle in the direction parallel to the mean magnetic field, one can use theoretical expressions that employ pitch-angle diffusion coefficients. In this work we review some of the methods used in estimating pitch-angle diffusion coefficients from test particle computer simulations. We examine if these methods and theoretical approaches are able to provide consistent estimates of the parallel mean free path, that can also be obtained directly from computer simulations. We perform test particle simulations for synthetic turbulence models over a range of turbulence parameters and particle energies. From the trajectories of test particles, pitch-angle distribution functions and statistics of pitch-angle displacements are obtained, which are then used to estimate the pitch-angle diffusion coefficients. We find that a method using the pitch-angle flux and derivative of the pitch-angle distribution is able to provide accurate values for the parallel mean free path over the range of parameters considered. Other methods considered are accurate only for a limited range of the turbulent fluctuation strength, or must be evaluated at a specific time to provide a reasonable estimate.

1. Introduction

The transport of energetic charged particles (or cosmic rays) in turbulent magnetic fields is an important concept in various astrophysical and laboratory plasma contexts. Typically one is interested in the spatial particle diffusion coefficients parallel and perpendicular to some large-scale mean magnetic field direction. The spatial diffusion coefficient parallel to the mean field (here taken to be in the z -direction) is typically expressed as

$$\kappa_{\parallel} = \lim_{t \rightarrow \infty} \frac{\langle (\Delta z)^2 \rangle}{2t}, \quad (1)$$

where $\Delta z(t)$ is the displacement of a particle in the parallel direction over a time t , and the angle brackets denote an ensemble average over particles. This diffusion coefficient is sometimes expressed in terms of the mean free path of a particle, λ_{\parallel} , which is related via $\kappa_{\parallel} = (v/3)\lambda_{\parallel}$, where v is the particle speed. An important quantity related to spatial diffusion is the pitch-angle Fokker-Planck coefficient (or pitch-angle diffusion coefficient), $D_{\mu\mu}(\mu)$, which depends on the pitch-angle cosine $\mu = \cos\theta$, where θ is the angle between the particle's velocity vector



and the mean magnetic field direction. Its relation to the parallel diffusion coefficient can be expressed as (e.g. [1])

$$\lambda_{\parallel} = \frac{3v}{8} \int_{-1}^1 \frac{(1 - \mu^2)^2}{D_{\mu\mu}(\mu)} d\mu, \quad (2)$$

which should be valid when the particle pitch-angle distribution function, $f(\mu, t)$, is almost isotropic. Parallel diffusion theory is dominated by the quasilinear theory [2] and its various extensions, which focus on obtaining expressions for $D_{\mu\mu}(\mu)$.

Test particle computer simulations are a useful tool in the study of charged particle transport, and in particular can be used to test theoretical expressions for particle diffusion coefficients. For test particle simulations, the parallel diffusion coefficient can be obtained as implied in equation (1), by simulating the trajectories of a large number of particles in turbulent magnetic fluctuations up to a sufficiently large time where $\langle(\Delta z)^2\rangle \propto t$, so that the ratio in the limit becomes constant. This occurs in most contexts where the magnetic field has a well-defined integral length scale. One could apply an analogous expression for the pitch-angle diffusion

$$D_{\mu\mu}(\mu) = \lim_{t \rightarrow \infty} \frac{\langle(\Delta\mu)^2\rangle}{2t}, \quad (3)$$

where $\Delta\mu = \mu(t) - \mu$ is the pitch-angle displacement from its initial value μ . However, this form has a severe difficulty in that μ is bounded, i.e. $\mu \in [-1, 1]$, so that $(\Delta\mu)^2 \leq 4$, and in the infinite limit one obtains $D_{\mu\mu}(\mu) = 0$. In the literature, this problem is remedied by taking the value of this expression at a sufficiently large time (see, e.g. [3]), or simply after one gyroperiod t_L of a particle, as suggested by [4]. An alternative approach to obtain $D_{\mu\mu}$ involves following the evolution of the pitch-angle distribution function $f(\mu, t)$ of the test particles and assume that it obeys a pitch-angle diffusion equation (and hence Fick's law), so that $D_{\mu\mu}$ can be calculated via the derivatives of f and the pitch-angle flux (e.g. [5–7]).

The aim of this work is to obtain a better understanding of how to calculate pitch-angle diffusion coefficients in test particle simulations. We compare the two approaches to calculating pitch-angle diffusion coefficients primarily for the widely-studied slab model, for which the original theory [2] and equation (2) are thought to apply, particularly when the turbulent fluctuations are weak compared with the background magnetic field. We additionally make comparisons for the two-component (composite) magnetic fluctuation model that has been used to describe the solar wind. We determine if there is an agreement between the parallel mean free path calculated from spatial diffusion coefficients, as in equation (1), and that obtained from the pitch-angle diffusion coefficients via equation (2). We also compare results with the appropriate quasilinear theory [8].

2. Computer simulations

We perform test particle simulations for two-component magnetic turbulence that are very similar to those of [9]. The slab model, which is the main focus of this work, simply neglects the second (two-dimensional) component. We constructed a periodic slab magnetic field, $(b_x^{\text{slab}}(z), b_y^{\text{slab}}(z), 0)$ in cartesian coordinates, on a one-dimensional grid of 2^{25} points, with a periodic box length of $80,000l_s$, where l_s is a parallel coherence scale associated with the slab power spectrum. A 2D component, $(b_x^{2D}(x, y), b_y^{2D}(x, y), 0)$, was constructed on a two-dimensional grid with 4096×4096 grid points. This represents a two-dimensional periodic box of size $100l_{2D} \times 100l_{2D}$, where l_{2D} is a perpendicular length scale. We take $l_s = l_{2D} = 1$ and characterise the relative strength of the two components with $f_s \in [0, 1]$, where $f_s = 1$ means all the magnetic energy is in slab fluctuations, and $f_s = 0$ implies purely 2D fluctuations. We consider only one case with $f_s \neq 1$, which corresponds to realistic solar wind parameters, but where the theory may be considered less accurate. The total magnetic field is given by

$\vec{B} = \vec{b} + B_0 \vec{z}$, where \vec{z} is the unit vector in the parallel (z) direction, and B_0 is the uniform mean field strength. Here \vec{b} is the turbulent field which is a sum of the 2D and slab components above. For each set of test particle simulations, we used several random realisations of both the 2D and slab components. The test particle trajectories $\vec{x}(t)$ were obtained by numerical integration of the Newton-Lorentz equations

$$\frac{d\vec{v}}{dt} = \alpha \vec{v} \times \vec{B}(\vec{x}[t]), \quad \frac{d\vec{x}}{dt} = \vec{v}, \quad (4)$$

where $\alpha = qB_0 l_s / (\gamma m v_0)$, with q the particle charge, γ the Lorentz factor, m the particle mass and v_0 the unit of velocity, which we take here for simplicity as $v_0 = 1$. The simulations can be varied in the parameters f_s , R_L/l_s and b/B_0 , where $b = |\vec{b}|$ and $R_L = \gamma m v_0 / (|q| B_0)$ is the particle's Larmor radius.

We used two types of initial pitch-angle ($\mu = v_z/|v|$) distributions as shown in panel (a) of figure 1. When calculating κ_{\parallel} we sampled pitch angles from an isotropic distribution, $f(\mu) = 1/2$, and when using pitch-angle diffusion coefficients we sampled from a linear distribution shifted towards positive μ values. The initial locations of the particles were sampled uniformly over the periodic boxes.

From particle trajectories that have an isotropic pitch-angle distribution at $t = 0$, we calculate the spatial diffusion coefficient κ_{\parallel} as described in Sect. 1, and from that obtain λ_{\parallel} . We also obtain an approximation for $D_{\mu\mu}(\mu)$ based on equation (3) by evaluating it after 1 gyroperiod t_L , which we denote $D_{\mu\mu}[\text{TL}]$.

From simulations starting with the initial pitch-angle distribution as in figure 1(a), we follow the evolution of $f(\mu, t)$ by constructing histograms with 80 bins, with bin centres at $\mu_j = -1 + (j - \frac{1}{2})\delta\mu$, $j = 1, 2, \dots, 80$, where $\delta\mu = 1/40$. Although we are using around 5×10^6 particles or more, it is necessary to smooth the histograms of $f(\mu, t)$ slightly so that $\partial f(\mu, t)/\partial\mu$ can be calculated numerically. We apply Gaussian smoothing in both the μ and t directions, then use a centred finite-difference approximation to calculate $\partial f(\mu, t_0)/\partial\mu$ at bin boundaries, where t_0 can be any time in the evolution of f . We calculate the pitch-angle flux at a given μ via $j(\mu, t_0) = [\int_{-1}^{\mu} f(\mu', t_2) d\mu' - \int_{-1}^{\mu} f(\mu', t_1) d\mu'] / (t_2 - t_1)$, where $t_1 = t_0 - \delta t$ and $t_2 = t_0 + \delta t$, with δt a sufficiently large time interval of order t_L or larger. Again, $j(\mu, t_0)$ is obtained at bin boundaries, and in practice must be calculated with discrete sums, rather than integrals. Then for a given t_0 we define

$$D_{\mu\mu}(\mu, t_0)[\text{FD}] = \frac{-j(\mu, t_0)}{\partial f(\mu, t_0)/\partial\mu}, \quad (5)$$

and then by considering different times $t_0 = t_i$ in the evolution of f we construct $D_{\mu\mu}(\mu)[\text{FD}] = \frac{1}{N} \sum_{i=1}^N D_{\mu\mu}(\mu, t_i)$, where N is the number of times over which the average is calculated. equation (5) is essentially the definition of a diffusion coefficient according to Fick's law. This approach is very similar to that used in [7]. In addition to the computational values, we also take a theoretical value corresponding to the second-order quasilinear theory of [8], which we denote $D_{\mu\mu}[\text{QL}]$.

3. Results

We considered 8 sets of parameters for the test particles, as summarised in the first three columns of table 1. Plots of corresponding $D_{\mu\mu}$ obtained with the various methods are shown in figure 1, panels (b)-(i). For pure slab cases with small b/B_0 and R_L , as in panels (b),(g) and (h), all methods show similar shaped $D_{\mu\mu}$, with $D_{\mu\mu}[\text{QL}]$ in very good agreement with $D_{\mu\mu}[\text{FD}]$. In the large R_L cases, and the composite case, $f_s = 0.2$, one of $D_{\mu\mu}[\text{QL}]$ or $D_{\mu\mu}[\text{TL}]$ deviates significantly from $D_{\mu\mu}[\text{FD}]$. In terms of the resulting λ_{\parallel} , obtained via equation (2) (replacing the integral with a discrete sum in the test particle cases), $D_{\mu\mu}[\text{FD}]$ is in excellent agreement

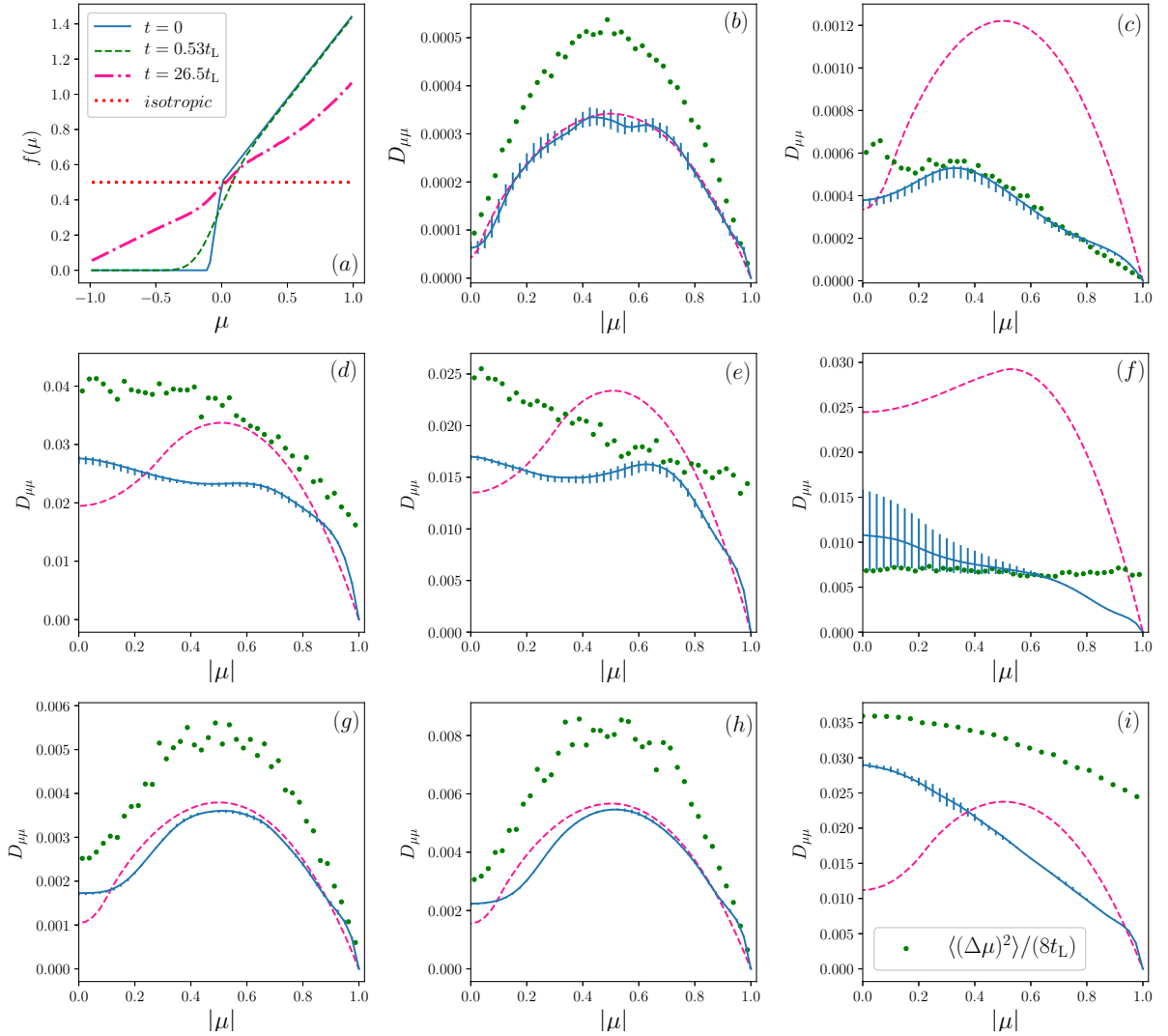


Figure 1. (a) shows the evolution of $f(\mu, t)$ in a test particle simulation. (b)-(i) correspond to the sequence of runs in table 1 and show $D_{\mu\mu}$ [FD] (solid lines), $D_{\mu\mu}$ [QL] (dashed lines) and $D_{\mu\mu}$ [TL] (dots). The vertical bars indicate the range of values over which the average $D_{\mu\mu}$ [FD] was obtained. Note that in panel (i), the dotted line has been obtained at $t = 4t_L$.

with the result obtained from spatial diffusion, as can be seen from the relative error shown in the final column of table 1. The result is slightly less impressive in the $f_s = 0.2$ case that includes 2D fluctuations, but still far more accurate than the other estimates.

4. Discussion and conclusions

We have compared two methods to calculate $D_{\mu\mu}$ from test particle simulations with theory and assessed their ability to predict λ_{\parallel} as given by spatial diffusion coefficients for the slab magnetic fluctuation model and for a special case of the two-component model. The method involving the pitch-angle flux and the μ -derivative of the distribution function $f(\mu, t)$ was found to be very accurate over the parameters considered. The quasilinear theory provides reasonable estimates for $b/B_0 \lesssim 0.3$, provided that R_L is not too large. The method using $(\Delta\mu)^2$ seems to work well only for a limited range of parameters, and $D_{\mu\mu}$ [TL] deviates significantly from $D_{\mu\mu}$ [FD] in the

Table 1. Comparison of the parallel mean free path (λ_{\parallel}) with estimates based on equation (5) (λ_{\parallel} [FD]), equation (3) (λ_{\parallel} [TL]) and the second-order quasilinear theory (λ_{\parallel} [QL]).

Label	f_s	b/B_0	R_L/l_s	λ_{\parallel}/l_s	λ_{\parallel} [FD]/ l_s	λ_{\parallel} [QL]/ l_s	λ_{\parallel} [TL]/ l_s	λ_{\parallel} [FD] error
(b)	1	0.03	0.1	2200.56	2189.72	2167.20	1362.14	0.0049
(a,c)	1	0.1	3.0	987.30	985.79	536.59	869.88	0.0015
(d)	1	0.3	0.1	14.82	14.70	15.85	10.64	0.0077
(e)	1	0.3	0.3	24.40	24.42	22.86	19.19	0.0001
(f)	1	0.5	3.0	42.42	42.04	15.45	58.61	0.0065
(g)	1	0.1	0.1	159.18	160.21	172.68	104.51	0.0089
(h)	1	0.1	0.03	117.00	117.06	115.06	72.49	0.0005
(i)	0.2	0.5	0.05	14.97	17.76	24.11	2.94	0.1861

composite turbulence case. Our results suggest that estimates based on $(\Delta\mu)^2$ may be generally quite inaccurate, even if an optimal evaluation time is found.

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