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Xinliang Gao, Quanming Lu & Shui Wang

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ORIGINAL ARTICLE

Dynamics of charged particles and perpendicular diffusion in turbulent magnetic field

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Abstract A test particle code is employed to explore the dynamics of charged particles and perpendicular diffusion in turbulent magnetic field, where a three-dimensional (3D) isotropic turbulence model is used in this paper. The obtained perpendicular diffusion at different particle energies is compared with that of the nonlinear guiding center (NLGC) theory. It is found that the NLGC theory is consistent with test particle simulations when the particle energies are small. However, the difference between the NLGC theory and test particle simulations tends to increase when the particle energy is sufficiently large, and the threshold is related to the turbulence bend-over length. In the NLGC theory, the gyrocenter of a charged particle is assumed to follow the magnetic field line. Therefore, when the particle has sufficiently large energy, its gyroradius will be larger than the turbulence bend-over length. Then the particle can cross the magnetic field lines, and the difference between the test particle simulations and NLGC theory occurs.

Keywords Turbulent magnetic field · Perpendicular diffusion · Test particle simulation · Nonlinear guiding center theory

X. Gao \cdot Q. Lu (\boxtimes) \cdot S. Wang

CAS Key Laboratory of Basic Plasma Physics, Department of Geophysics and Planetary Science, University of Science and Technology of China, Hefei 230026, China e-mail: qmlu@ustc.edu.cn

X. Gao

State Key Laboratory of Space Weather, Chinese Academy of Sciences, Beijing 100190, China

1 Introduction

The diffusion of charged particles in turbulent magnetic field is being attracted more and more attentions due to its relation with the cosmic ray transport (Jokipii et al. 1993; Matthaeus et al. 1995, 2003; Giacalone and Jokipii 1999; Mace et al. 2000; Zank et al. 2004; Shalchi 2006, 2009; Shalchi and Dosch 2008; Tautz 2010). Since 1960s, different approaches have been attempted to solve the problem of the cosmic ray diffusion in turbulent magnetic field. The first attempt is the classical quasi-linear theory (QLT) developed by Jokipii (1966) to study the diffusion of charged particles in a slab model of turbulent magnetic field, which can only describe the diffusion along the mean magnetic field properly. The field line random walk (FLRW) theory (Jokipii 1966; Matthaeus et al. 1995) was emerged from QLT and assumed that the gyrocenter of a charged particle follows the magnetic field line. The diffusion perpendicular to the mean magnetic field is governed by the diffusive spread of the magnetic field lines. The perpendicular diffusion of the FLRW theory does not agree with that of test particle simulations for both low- and high-energy charged particles (Giacalone and Jokipii 1999; Mace et al. 2000; Qin et al. 2002a, 2002b). An important step to understand the perpendicular diffusion was the nonlinear guiding center (NLGC) theory developed by Matthaeus et al. (2003). Although the gyrocenter of a charge particle is still assumed to follow the magnetic field line, the influence of parallel scattering, as well as dynamical turbulence, on the perpendicular diffusion is considered. Although the perpendicular diffusion of the NLGC theory behaves well for a wide range of particle energies, it has problems to explain subdiffusive transport for slab turbulence and other limits. Shalchi (2010) further developed a unified particle diffusion theory for cross-field scattering, and the new theory can explain subdiffusive transport for slab turbulence and recovery of the diffusion for slab/twodimensional (2D) and three-dimensional (3D) turbulence.

In this paper, a test particle code is employed to investigate the perpendicular diffusion in turbulent magnetic field, where a 3D isotropic turbulence model is used. The obtained perpendicular diffusion at different particles energies are compared with that of the NLGC theory, and the physical mechanism for the difference is also explained in this paper.

2 Simulation model

The turbulent magnetic field can be written as $\mathbf{B}(x, y, z) = B_0 \hat{\mathbf{z}} + \delta \mathbf{B}(x, y, z)$, where $B_0 \hat{\mathbf{z}}$ is the mean magnetic field. A three-dimensional realization of the magnetic field is attained by summing over a large number of plane waves with a spherically symmetric propagation direction, and with random polarizations and phases. It is shown that the turbulent part is isotropic and spatially homogeneous in the limit of an infinite number of wave modes (Batchlor 1960). The disturbance component is expressed as follows:

$$\delta \mathbf{B}(x, y, z) = \sum_{n=1}^{N_m} A(k_n) \hat{\boldsymbol{\xi}}_n \exp(ik_n z'_n + i\beta_n) \tag{1}$$

where

$$\hat{\boldsymbol{\xi}}_n = \cos \alpha_n \hat{\mathbf{x}}'_n + i \sin \alpha_n \hat{\mathbf{y}}'_n \tag{2}$$

and

$$\begin{pmatrix} x'\\ y'\\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta_n \cos\phi_n & \cos\theta_n \sin\phi_n & -\sin\theta_n\\ -\sin\phi_n & \cos\phi_n & 0\\ \sin\theta_n \cos\phi_n & \sin\theta_n \sin\phi_n & \cos\theta_n \end{pmatrix} \begin{pmatrix} x\\ y\\ z \end{pmatrix}$$
(3)

In (2) and (3), $A(k_n)$ represents the amplitude of the wave mode *n*, with wave-number k_n , polarization α_n , and phase β_n . The propagation direction of each mode is defined by the angles θ_n and ϕ_n in (3) (Giacalone and Jokipii 1999).

The amplitude function $A(k_n) \propto \sqrt{G(k_n)}$ is related to the turbulence spectrum $g(k_n)$ (Tautz et al. 2006), which gives:

$$A^{2}(k_{n}) = \delta B^{2} G(k_{n}) \left[\sum_{n=1}^{N_{m}} G(k_{n}) \right]^{-1}$$
(4)

where $G(k_n) = G_0 g(k_n) \equiv G_0 (1 + k_n^2 L_c^2)^{-\nu}$, $\nu = \gamma/2$ and L_c is the bend-over length. δB^2 is the wave variance, and γ is the spectral index of the turbulence. And

$$G_0 = 4\delta B^2 L_c C(\nu) \tag{5}$$

In (5), C(v) is a normalization factor. Both C(v) and γ are dependent on the dimensionality of the turbulence. We

choose a logarithmic spacing in k_n so that $\Delta k_n/k_n$ is a constant (Giacalone and Jokipii 1999), where Δk_n is the difference between the k_n . A 3D isotropic model for turbulence is used. In the isotropic model, the wave modes have wave vectors distributed randomly in direction and with random phases and polarizations. The spectral index is $\gamma = 5/3$, and a total of 300 wave modes are used in this paper. The amplitude of the turbulence is

$$\sum_{n=1}^{N_m} B_k^2 / B_0^2 = 1.0.$$

The particle trajectories can be computed by numerically integrating the Lorentz force on each particle, which is given by:

$$\frac{d\mathbf{v}}{dt} = \frac{q}{m}\mathbf{v} \times \mathbf{B} \tag{6}$$

where q is the charge, m is the mass, and \mathbf{v} is the particle velocity.

In the simulations, we follow trajectories of 1000 particles. The time step is chosen as $\Omega \Delta t = 0.05$ (where $\Omega =$ qB_0/m is the gyrofrequency based on the mean magnetic field). When the Lorentz force is integrated, the magnetic field is generated anew for each step (Giacalone and Jokipii 1999; Tautz 2010). The advantage is that the magnetic field has to be calculated only where it is actually needed. The alternative method is to specify the magnetic field on a discrete spatial lattice (Qin et al. 2002a, 2002b), which is more time-consuming owing to the fact that too many lattice points are needed to make the computation sufficiently accurate. The Bulirsh-Stoer method, which is described in detail by Press et al. (1986), is used in this paper to integrate the particle trajectories. It is highly accurate and conserves energy. The alternative method is to use the Pedian simulation code developed by Tautz (2010).

3 Simulation results

Figure 1 illustrates the power spectrum that is used to generate the magnetic fluctuations. Note that the power spectrum is zero above the upper cut-off or below the lower cut-off, as indicated in the figure. The lower and upper cut-offs are $kL_c = 10^{-3}$ and $kL_c = 2.608 \times 10^4$, respectively.

The diffusion tensor defined in terms of the Fokker-Planck coefficients can be calculated with the mean square displacements of all possible particle trajectories (Giacalone and Jokipii 1994), which can be described as:

$$\kappa_{ij} = \frac{\langle \Delta r_i \, \Delta r_j \rangle}{2\Delta t} \tag{7}$$



Fig. 1 The power spectrum of the 3D isotropic turbulence used in the numerical simulations. Note that the power spectrum is identically zero above the upper cut-off or below the lower cut-off, as indicated in the figure

where $\Delta \mathbf{r}$ is the displacement of a particle from its original position after a time Δt . The angle brackets denote ensemble averages, which can also be viewed as averages over many particle trajectories. The definition reads

$$\langle \Delta r_i \Delta r_j \rangle = \frac{1}{N} \sum_{i=1}^N \Delta r_i \Delta r_j \tag{8}$$

where N is the number of the particles (Giacalone and Jokipii 1994).

However, as pointed out by Shalchi (2011) that the diffusion coefficient based on (7) is only valid for the in-diagonal elements. For the off-diagonal elements, a time integral over the velocity correlation function should be used. In our paper, we only consider the perpendicular diffusion coefficient, which belongs to in-diagonal elements. Therefore, it will not change our calculations.

At first the perpendicular displacement of the particles is calculated according to (8), and then we can calculate its slope as the perpendicular diffusion coefficient. Figure 2 shows the evolution of the perpendicular diffusion coefficient k_{\perp} for particles with the velocity $1.0L_c\Omega$. The particles are diffusive and at last the diffusion coefficient can reach an asymptotic value. We choose the asymptotic value, which is about $0.1927L_c\Omega$, as the final perpendicular diffusion coefficient. All the perpendicular diffusion coefficients in this paper are obtained with this method.

Figure 3 compares the perpendicular diffusion coefficients k_{\perp} obtained from test particle simulations and the NLGC theory. Figure 3(a) describes the perpendicular diffusion coefficients at different energies, which are calculated



Fig. 2 The evolution of the perpendicular diffusion coefficient k_{\perp} for particles with the velocity $1.0L_c\Omega$. The 3D isotropic turbulence model with the power spectrum as described in Fig. 1 is used to calculate the perpendicular diffusion coefficient



Fig. 3 (a) The perpendicular diffusion coefficients obtained from test particle simulations (*solid line*) and the NLGC theory (*dotted line*). (b) The difference of the perpendicular diffusion coefficients between the test particle simulations and the NLGC theory. The 3D isotropic turbulence model with the power spectrum as described in Fig. 1 is used to calculate the perpendicular diffusion coefficients

with test particle simulations (solid line) and the NLGC theory (dotted line), respectively, while Fig. 3(b) plots their difference (the coefficients of test particle simulations minus Author's personal copy



Fig. 4 Particle trajectories (*red line*) superimposed on magnetic field lines (*black line*) when the particle velocity is high $(1.0L_c\Omega)$, and r_g is the gyroradius. The magnetic field lines are calculated with the 3D isotropic turbulence model with the power spectrum as described in Fig. 1



Fig. 5 Particle trajectories (*red line*) superimposed on magnetic field lines (*black line*) when the particle velocity is small $(0.05L_c\Omega)$, and r_g is the gyroradius. The magnetic field lines are calculated with the 3D isotropic turbulence model with the power spectrum as described in Fig. 1

that of the NLGC theory). The perpendicular diffusion coefficients of the NLGC theory are calculated based on the integral equation given in Appendix C of Tautz et al. (2006) with the parameter $a^2 = 1$, and the equation is solved with a iteration process. The perpendicular diffusion coefficients become large with the increase of the energy. The results show that the NLGC theory can describe the perpendicular diffusion very well at low and medium energies. However, there exists a difference between test particle simulations and the NLGC theory at higher energies, and the difference increases when the particle velocity is larger than about $1.0L_c\Omega$ (we define this velocity as the beginning velocity). At the same time, the gyroradius of the particle is larger than $1.0L_c$. When the particle velocity is sufficiently large (larger than 4.0 $L_c\Omega$), the perpendicular diffusion of the test particle simulations is about 2 times that of the NLGC theory. Therefore, we speculate that there may be a relation between the beginning velocity and bend-over length. When the gyroradius of a particle exceeds the bend-over length, the power of the waves which can resonantly interact with the particle become sufficiently large, and then the particle can cross the magnetic field lines. This can be demonstrated in Fig. 4, which shows typical particle trajectories in the (x, y) plane. Figure 4 shows a typical particle trajectory with the velocity $1.0L_c\Omega$, and Fig. 5 plots a typical particle trajectory with the velocity $0.05L_c\Omega$. The magnetic field lines in the (x, y)plane (black lines) are also plotted in the figures. It is shown that the low-energy particle will follow the initial magnetic field line. However, the high-energy particle can cross the magnetic field lines; therefore, its perpendicular diffusion will be different from that of the NLGC theory since the gyrocenter of a charge particle is assumed to follow the magnetic field line in the NLGC theory. Our simulation results are consistent with the theoretical prediction by Shalchi and Dosch (2008). In their theory the assumption that the gyrocenter of a particle follows the magnetic field line is replaced by the Newton-Lorentz equation. They also found that when the particle gyroradius is larger than the bend-over length, the predicted perpendicular diffusion is about 2 times that of the NLGC theory.

4 Discussion and conclusions

The charged particle perpendicular diffusion coefficient is an important parameter for the theoretical description of various physical problems. In our paper, we compare the particle perpendicular diffusion coefficients obtained from test particle simulations with that from the NLGC theory, and a 3D isotropic turbulence model is used. The NLGC theory can describe the diffusion very well when the particle velocity is not so high. When the particle velocity reaches the beginning velocity ($\sim 1.0L_c\Omega$), there is a difference between the NLGC theory and test particle simulations, and it tends to increase with the particle velocities. This difference is related to the turbulence bend-over length. Our explanation is that when the particle velocities reach the beginning velocity, their resonant scattering by the waves with the larger amplitude contributes more and more to the perpendicular Author's personal copy

diffusion. Then, many particles start to escape from their initial magnetic field lines, and cross over them. Therefore, the assumption in the NLGC theory that the gyrocenter of a particle follows the magnetic field line is not reasonable when the particle energy is sufficiently large.

In the heliosheath, the amplitude of the magnetic field is about 0.1 nT (Burlaga et al. 2005). The difference of the perpendicular diffusion coefficients between test particle simulations and the NLGC theory becomes obvious, when the bend-over length of the turbulence is smaller than about 0.01 and 0.1 AU for protons with the energies of 1 and 100 MeV, respectively. These are reasonable values in the heliosheath.

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