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NONLINEAR PARALLEL DIFFUSION OF CHARGED PARTICLES: EXTENSION TO THE NONLINEAR GUIDING CENTER THEORY

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ABSTRACT

A nonlinear theory of the parallel diffusion of charged particles with perpendicular scattering and dynamical turbulence is obtained. The combination of the new parallel diffusion theory and the nonlinear guiding center theory shows good agreement with numerical simulations using typical parameters for a solar wind. Furthermore, the combination of the theories has a simpler mathematical form and is more computationally tractable than the weakly nonlinear theory.

Subject headings: cosmic rays — diffusion — turbulence

1. INTRODUCTION

The diffusion of energetic particles in magnetic fluctuations is very important in both solar physics and stellar physics. A better understanding of this problem can help to describe the transport of solar energetic particles. Knowledge of the diffusion tensor is required to study the modulation of cosmic rays (Parker 1965). Furthermore, the diffusive acceleration of high-energy particles by collisionless shock in the heliosphere of a star, as well as in the stellar wind, is based on the theory of scattering and transport of energetic particles (Bell 1978; Forman & Webb 1985). Jokipii (1966) provided a classical quasi-linear theory (QLT) for a charged particle's diffusion in a slab model of magnetic turbulence. QLT assumes the gyrocenters of charged particles follow magnetic field lines, and the diffusion coefficients perpendicular and parallel to the large-scale mean magnetic field $\boldsymbol{B}_0$ can be calculated separately. Palmer (1982) showed that the observed parallel scattering is usually much smaller than the result from QLT. Bieber et al. (1994) suggested that when extended to include some effects of more realistic turbulence (e.g., slab + two-dimensional [2D] composite magnetic turbulence model), QLT can describe parallel diffusion well. However, Qin (2002) and Qin et al. (2002b) showed that QLT results do not agree with simulations for parallel diffusion of medium- and low-energy charged particles in composite turbulence. Furthermore, although it can be demonstrated that there is no parallel scattering in 2D magnetic turbulence in QLT, a finite parallel diffusion coefficient can be obtained in numerical simulations (Qin et al. 2006).

The perpendicular diffusion of charged particles has been a puzzle for a very long time, and heliospheric observations suggesting both decreased and enhanced transverse diffusion have been reported (Mazur et al. 2000; Maclennan et al. 2001). The field line random walk (FLRW) theory emerged from QLT by using a composite turbulence model to calculate the perpendicular diffusion coefficient (Jokipii 1966; Matthaeus et al. 1995). There have also been other attempts to calculate the perpendicular diffusion coefficient, namely, theories such as BAM (Bieber & Matthaeus 1997) and CC&RR (Rechester & Rosenbluth 1978; Stix 1978; Chandran & Cowley 1998). However, none of the above theories agree with the simulation results of perpendicular diffusion for both low- and high-energy charged particles (Giacalone & Jokipii 1999; Mace et al. 2000; Qin et al. 2002a, 2002b). The nonlinear guiding center theory (NLGC; Matthaeus et al. 2003) is the first perpendicular diffusion theory to agree well with simulations. NLGC is derived from the Taylor-Green-Kubo (TGK) formulation (e.g., Kubo 1957) by assuming that transverse complexity decorrelates trajectories after parallel scattering, so the parallel diffusion coefficient is input to calculate the perpendicular diffusion coefficient. For closure, the parallel diffusion coefficients are obtained from other theories (e.g., QLT) or simulation results; therefore, it becomes essential to develop a theory of parallel diffusion with nonlinear effects. Hinted by NLGC, Shalchi et al. (2004) developed the weakly nonlinear theory (WNLT) to calculate perpendicular and parallel diffusion coefficients simultaneously. WNLT is based on QLT with nonlinear extensions that consider the movement of the guiding centers perpendicular to the background field.

Both NLGC, with simulation results of parallel diffusion coefficients as input, and WNLT provide theoretical results of perpendicular diffusion coefficients with good agreement with simulations. Furthermore, WNLT is more complete, since it provides theoretical results for parallel diffusion coefficients, which are in good agreement with simulations too. However, compared to NLGC, WNLT is very mathematically complicated and difficult to apply to varied turbulence models. So in practice, to study the diffusion of a charged particle theoretically, one would still use NLGC with a parallel diffusion coefficient from QLT as input (e.g., Shalchi et al. 2006; Shalchi & Schlickeiser 2006).

In this paper, applying similar approximations to those used in the derivation of NLGC, we develop a parallel diffusion theory considering nonlinear effects, the nonlinear parallel diffusion theory (NLPA), starting from the method used to calculate the pitch-angle diffusion coefficient by Jokipii (1966). The extended nonlinear guiding center theory (NLGC-E) is obtained by combining the NLGC and NLPA. From NLGC-E, the perpendicular and parallel diffusion coefficients can be determined simultaneously, just as they can from WNLT, but NLGC-E has a simpler mathematical form and can be easily applied to various turbulence models. We can also show that the NLGC-E agrees well with numerical simulations using parameters from a typical solar wind.

Note that in the models of the particles' diffusion coefficients considered in this paper, we assume a uniform large-scale background field with a superposed turbulent magnetic field. To study the effect of the different length scales and timescales, G. Webb and coauthors (e.g., Webb et al. 2003) proposed parallel particle transport models with multiscale analysis in quasi-periodic flows.

Although the approach by Webb et al. (2003) does not describe the transport of particles in a turbulent medium, it is assumed that in their models turbulent diffusion coefficients can be obtained by ensemble averaging over random and periodic structures with small correlation lengths.

2. DERIVATION OF THE NONLINEAR PARALLEL DIFFUSION THEORY

In order to calculate the pitch-angle diffusion coefficient of particles in magnetic fluctuations, we start with the definition of the cosine of the pitch angle $\mu = v_z/v = \boldsymbol{B}_0 \cdot \boldsymbol{v}/(B_0 v)$, where $\boldsymbol{B}_0 = B_0 \hat{\boldsymbol{e}}_z$ is the large-scale averaged magnetic field. A change of μ is then evaluated as (Jokipii 1966)

$$\begin{aligned}\Delta\mu(t) &= \frac{\Omega}{B_0 v}\int_0^t \hat{\boldsymbol{z}} \cdot (\boldsymbol{v} \times \boldsymbol{b})\, d\tau \\ &= \frac{\Omega}{B_0 v}\int_0^t (v_x b_y - v_y b_x)\, d\tau, \qquad (1)\end{aligned}$$

where v is the particle's speed and $\Omega = eB_0/\gamma m_0 c$ is the unperturbed gyrofrequency. We also assume a statistically homogeneous magnetic field $\boldsymbol{B} = B_0 \hat{\boldsymbol{e}}_z + \boldsymbol{b}$, with magnetic fluctuations $\boldsymbol{b}$ perpendicular to $\boldsymbol{B}_0$, and that the electric field is negligible in the solar wind frame. The pitch-angle diffusion coefficient $\phi(\mu)$ can be calculated as

$$\phi(\mu) = \frac{\left\langle (\Delta\mu)^2 \right\rangle}{t}, \qquad (2)$$

where $\langle \ldots \rangle$ indicates the ensemble average. To proceed, we employ a series of approximations as follows.

First, we assume $t \to \infty$. Second, we assume that the fluctuations of the magnetic field and the particle's velocity are stationary and homogeneous on a large spatial and temporal scale. Therefore,

$$\begin{aligned}&\left\langle \frac{1}{t}\int_0^t dt' \int_{-t'}^{t-t'} d\tau\, v_\alpha(t') v_\beta(t'+\tau) b_\gamma(t') b_\delta(t'+\tau) \right\rangle \\ &\quad = \int_{-\infty}^{\infty} d\tau \left\langle v_\alpha(0) v_\beta(\tau) b_\gamma(0) b_\delta(\tau) \right\rangle, \qquad (3)\end{aligned}$$

where α, β, γ, and δ are x or y. In addition, we assume that the particle velocities are uncorrelated with the local magnetic field (Matthaeus et al. 2003). Thus, the fourth-order correlation is written as a product of second-order correlations, $\left\langle v_\alpha(0) v_\beta(\tau) b_\gamma(0) b_\delta(\tau)\right\rangle = \left\langle v_\alpha(0) v_\beta(\tau)\right\rangle \left\langle b_\gamma(0) b_\delta(\tau)\right\rangle$. Furthermore, we assume vanishing magnetic helicity, i.e., $\left\langle b_\gamma(0) b_\delta(\tau)\right\rangle = 0$ if $\gamma \neq \delta$. The pitch-angle diffusion coefficient $\phi(\mu)$ thus becomes

$$\phi(\mu) = 2\left(\frac{\Omega}{B_0 v}\right)^2 \int_{-\infty}^{\infty} d\tau \langle v_x(0) v_x(\tau)\rangle \left\langle b_y(0) b_y(\tau)\right\rangle. \qquad (4)$$

Next we assume that when the particles are scattered while traveling along the magnetic field lines, their velocity direction will be lost, so the two-time autocorrelation of parallel and perpendicular velocities has similar parallel scattering effects. Since the perturbed parallel velocity autocorrelation is assumed to be (Matthaeus et al. 2003)

$$\langle v_z(0) v_z(t')\rangle = \frac{v^2}{3} e^{-vt'/\lambda_\parallel}, \qquad (5)$$

we assume that the perturbed perpendicular one in pure slab-mode turbulence can be written as

$$\langle v_x(0) v_x(t')\rangle = \frac{1-\mu^2}{2} v^2 \cos(\Omega t') e^{-vt'/\lambda_\parallel}. \qquad (6)$$

Both of these two autocorrelation assumptions reduce to an unperturbed one without parallel scattering. Note that for the parallel velocity autocorrelation equation (5), the isotropic form is used, while for the perpendicular one, equation (6), we use the anisotropic form. Alternatively, we could use the isotropic form in equation (6) by replacing $1-\mu^2$ with $\frac{2}{3}$; however, we get similar results by doing so. Here we ignore the influence of perpendicular scattering on both of the velocity autocorrelation functions, considering that the timescale for the parallel diffusion to set up is much shorter than that for the (secondary) perpendicular diffusion to act (Qin et al. 2002b). Now we assume the perpendicular velocity autocorrelation in a composite model of turbulence can be written as

$$\langle v_x(0) v_x(t')\rangle = a_x \frac{1-\mu^2}{2} v^2 \cos(\Omega t') e^{-vt'/\lambda_\parallel}, \qquad (7)$$

where

$$a_x = \sqrt{\frac{\tilde{E}_s}{[\xi/(1+\xi)](1/\tilde{b}) + \tilde{b}/2\xi}}, \qquad (8)$$

with $\tilde{r} = 2\pi r_{\rm L}/\lambda_c$, $\tilde{b} = b/B_0$, $\xi = \tilde{r}/\tilde{b}$, $\tilde{E}_s = E_{\rm slab}/(E_{\rm slab} + E_{\rm 2D})$, and λ_c is the correlation length of the slab turbulence. Here equation (8) is an assumption with the following considerations. Since in turbulence with some transverse structure the perpendicular velocity autocorrelation would decrease over gyroperiods, and in the extreme case of pure 2D turbulence it vanishes long before parallel scattering occurs, we can assume that in a composite model turbulence the perpendicular velocity autocorrelation is proportional to the ratio $b_{\rm slab}/b_{\rm tot} \equiv (E_{\rm slab}/E_{\rm tot})^{1/2}$. Furthermore, for weaker turbulence with increased gyroradius, particles would sample more fluctuations in a gyroperiod. On the other hand, for stronger turbulence with increasing turbulence level, particles would experience more variations in the local magnetic field in a gyroperiod. Note that the above perpendicular velocity autocorrelation model is not valid in the very short timescale, $vt'/\lambda_\parallel \to 0$. However, we assume the approximation is acceptable, and we can check the final formula by comparing it with numerical simulations.

Still following Matthaeus et al. (2003), we model the Lagrangian magnetic autocorrelation $\left\langle b_y[\boldsymbol{x}(0), 0] b_y[\boldsymbol{x}(t'), t']\right\rangle$ by treating $\boldsymbol{x}(t')$ as a random variable and employing Corrsin's independence hypothesis (Corrsin 1959; Salu & Montgomery 1977; McComb 1990); as a result we have

$$\begin{aligned}&\left\langle b_y[\boldsymbol{x}(0), 0] b_y[\boldsymbol{x}(t'), t']\right\rangle \\ &\quad = \int d^3\boldsymbol{k}\, S_{xx}(\boldsymbol{k}) \Gamma_{xx}(\boldsymbol{k}, t') e^{-k_\perp^2 \kappa_{xx} t' - k_\parallel^2 \kappa_{zz} t'}, \qquad (9)\end{aligned}$$

where $S_{xx}(\boldsymbol{k}, t') = S_{xx}(\boldsymbol{k})\Gamma_{xx}(\boldsymbol{k}, t')$ is the magnetic turbulence spectral amplitude, $k_\perp^2 = k_x^2 + k_y^2$, and $k_\parallel = k_z$. Note that to obtain equation (9), Matthaeus et al. (2003) also assumed that the components of the trajectory have uncorrelated axisymmetric Gaussian distributions and that the distribution of displacements is diffusive for all values of time.

With the above assumptions, equation (4) becomes

$$\phi(\mu) = 2a_x\Omega^2(1-\mu^2)\int d^3\boldsymbol{k}\,\frac{S_{xx}(\boldsymbol{k})}{B_0^2} \times \int_0^\infty \frac{\cos(\Omega\tau)\Gamma(\boldsymbol{k},\tau)}{e^{\left(v/\lambda_\parallel + k_\perp^2\kappa_{xx} + k_\parallel^2\kappa_{zz}\right)\tau}}\,d\tau. \tag{10}$$

For simplicity we can further assume $\Gamma(\boldsymbol{k},\tau) = e^{-\gamma(\boldsymbol{k})\tau}$, and the above equation becomes

$$\phi(\mu) = 2a_x\Omega^2\left(1-\mu^2\right) \times \int d^3\boldsymbol{k}\,\frac{S_{xx}(\boldsymbol{k})}{B_0^2}\,\frac{v/\lambda_\parallel + k_\perp^2\kappa_{xx} + k_\parallel^2\kappa_{zz} + \gamma(\boldsymbol{k})}{\Omega^2 + \left[v/\lambda_\parallel + k_\perp^2\kappa_{xx} + k_\parallel^2\kappa_{zz} + \gamma(\boldsymbol{k})\right]^2}. \tag{11}$$

Since $\lambda_\parallel = (3v/4)\int_{-1}^{+1} d\mu\,(1-\mu^2)^2/\phi(\mu)$, we have

$$\lambda_\parallel = \left\{2a_x\frac{\Omega^2}{v}\int d^3\boldsymbol{k}\,\frac{S_{xx}(\boldsymbol{k})}{B_0^2}\,\frac{v/\lambda_\parallel + k_\perp^2\kappa_{xx} + k_\parallel^2\kappa_{zz} + \gamma(\boldsymbol{k})}{\Omega^2 + \left[v/\lambda_\parallel + k_\perp^2\kappa_{xx} + k_\parallel^2\kappa_{zz} + \gamma(\boldsymbol{k})\right]^2}\right\}^{-1}, \tag{12}$$

where a_x is defined by equation (8). Let us call the theoretical formula of the parallel diffusion coefficient obtained here NLPA and combine the two theories, NLGC and NLPA, to extend the nonlinear guiding center theory. We can solve the extended NLGC, i.e., NLGC-E, to obtain the parallel and perpendicular diffusion coefficients simultaneously, similar to Shalchi et al. (2004) with WNLT. However, we can see that NLGC-E has a much simpler mathematical form and is much more tractable than WNLT.

3. NUMERICAL SIMULATION RESULTS

In order to check the accuracy of NLGC-E for a static [$\gamma(\boldsymbol{k}) = 0$] two-component, slab/2D model magnetic field (Bieber et al. 1996) with a spectral index $\nu = \frac{5}{6}$, we compare the results from NLGC-E and numerical simulations that follow the trajectories of test particles. Besides the results from NLGC-E, QLT, and FLRW, we also show perpendicular mean free paths from NLGC with parallel mean free paths input from QLT or simulation results, denoted by NLGC-Q or NLGC-S, respectively. Some simulations with similar parameters were reported previously (Qin 2002; Qin et al. 2002b; Matthaeus et al. 2003; Shalchi et al. 2004). The spectral amplitude of a two-component model magnetic turbulence is chosen as (Bieber et al. 1996; Mace et al. 2000)

$$S_{xx}(\boldsymbol{k}) = S_{xx}^{2\mathrm{D}}(k_\perp)\frac{2k_y^2}{\pi k_\perp^3}\delta\left(k_\parallel\right) + S_{xx}^{\mathrm{slab}}\left(k_\parallel\right)\frac{\delta(k_\perp)}{2\pi k_\perp}, \tag{13}$$

where $S_{xx}^{\alpha}(k_\beta) = C(\nu)\lambda_\alpha\langle b_\alpha^2\rangle(1+k_\beta^2\lambda_\alpha^2)^{-\nu}$, with symbols (α,β) being either $(2\mathrm{D},\perp)$ or $(\mathrm{slab},\parallel)$ and $C(\nu) = (2\pi^{1/2})^{-1}\Gamma(\nu)/\Gamma(\nu-1/2)$. The correlation length of the slab turbulence is thus written as $\lambda_c = 2\pi C(\nu)\lambda_{\mathrm{slab}}$. If not mentioned otherwise, we use the following set of parameters in the simulations. We choose $\lambda_{\mathrm{slab}} = 10\lambda_{2\mathrm{D}}$ to guarantee diffusive perpendicular transport because of strong transverse complexity. The slab-mode turbulence is generated with 2^{22} Fourier modes in a periodic box of size $10^4\lambda_{\mathrm{slab}}$. The 2D mode turbulence is generated with 4096×4096 Fourier modes in a box of size $10^2\lambda_{\mathrm{slab}}$. The turbulence ultrascale (Matthaeus et al. 1995) of the model turbulence generated has a value of $\tilde{\lambda} = 1.02\lambda_{\mathrm{slab}}$. The energy in different turbulence components is controlled by the ratio $E_{\mathrm{slab}}/E_{\mathrm{tot}} \equiv E_{\mathrm{slab}}/(E_{\mathrm{slab}}+E_{2\mathrm{D}})$. The details of the methods of numerical simulations and calculation of diffusion coefficients from simulation results were described previously (Mace et al. 2000; Qin 2002; Qin et al. 2002a, 2002b). We choose the constant factor $a^2 = \frac{1}{3}$ in NLGC to get the best agreement between theoretical and simulation results (Matthaeus et al. 2003).

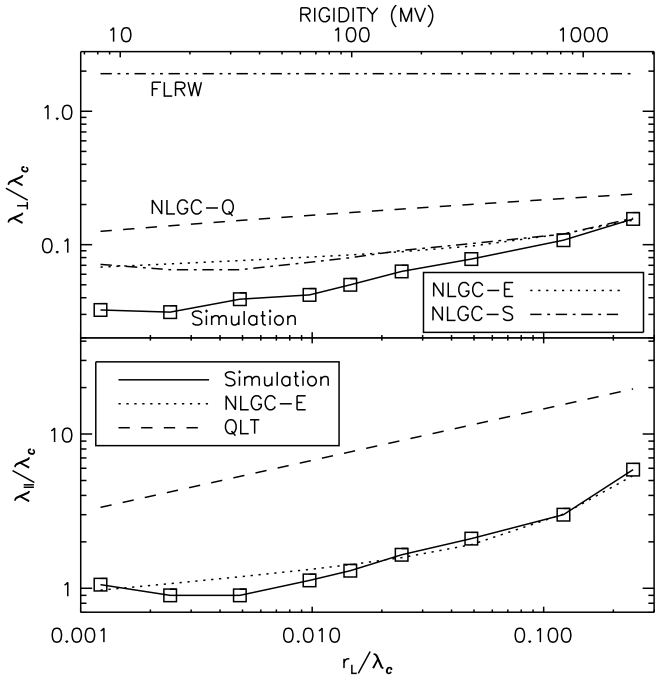

FIG. 1.—Perpendicular (*top*) and parallel (*bottom*) mean free paths as a function of r_{L}/λ_c, with $b/B_0 = 1$ and $E_{\mathrm{slab}}:E_{2\mathrm{D}} = 20:80$. Rigidity of protons is also shown as the secondary horizontal axis by assuming $\lambda_c = 0.03$ AU and $B_0 = 5$ nT.

Figure 1 shows a comparison between simulations (*squares*) and several theoretical results, NLGC-E (*dotted line*) in both panels, QLT (*dashed line*) in the bottom panel, and NLGC-Q (*dashed line*, *top*), NLGC-S (*dash-dotted line*), and FLRW (*dot-dot-dashed line*) in the top panel, as a function of the ratio of gyroradius to the parallel correlation length r_{L}/λ_c for strong turbulence, $b/B_0 = 1$ and $E_{\mathrm{slab}}:E_{2\mathrm{D}} = 20:80$. As a secondary horizontal axis, we also show the protons' rigidity, considering typical turbulence in the solar wind at 1 AU by assuming $B_0 = 5$ nT and $\lambda_c = 0.03$ AU. From the figure we can see that for nearly 2 orders of magnitude of rigidity, or in the range of $[10, 2000]$ MV for protons within 1 AU, NLGC-E agrees much better than QLT or NLGC-Q for relatively strong turbulence. Since the parallel mean free paths from NLGC-E agree with simulations very well, perpendicular ones from NLGC-E agree with NLGC-S very well too. In addition, it is obvious that FLRW is the worst theory for perpendicular diffusion in the parameters given. Note that the rigidity range of protons we discuss here matches that of spacecraft observations in Palmer (1982) and Bieber et al. (1994).

Another series of simulation results in relatively weaker turbulence ($b/B_0 = 0.2$) with similar parameters is shown in Figure 2. Here it is seen that for higher rigidity particles, $r_{\mathrm{L}}/\lambda_c > 0.04$, QLT and NLGC-Q agree with simulations well for parallel and perpendicular mean free paths, respectively. On the other hand, for lower rigidity particles ($r_{\mathrm{L}}/\lambda_c < 0.04$) both QLT and NLGC-Q do not agree with simulations for parallel and perpendicular mean free paths, respectively. However, NLGC-E generally agrees well

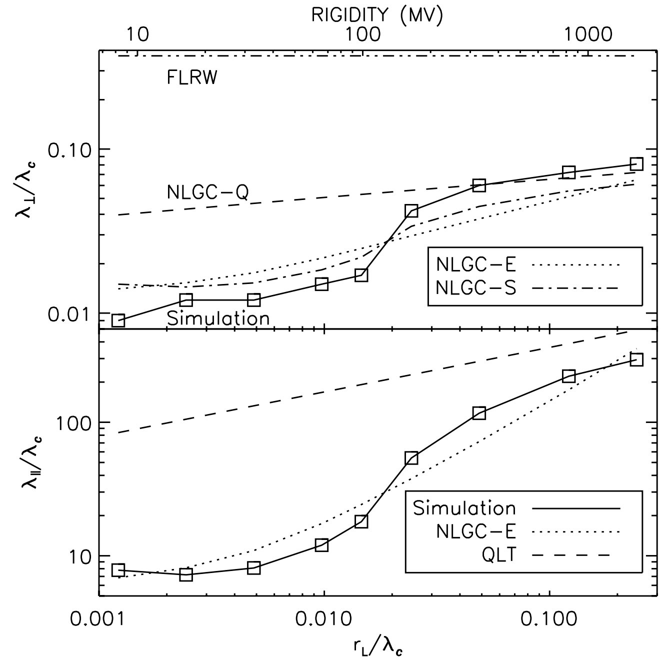

FIG. 2.—Same as Fig. 1, but for $b/B_0 = 0.2$.

with simulations for perpendicular and parallel mean free paths for $r_{\rm L}/\lambda_c$ in the range of $[0.001, 0.2]$. Again, for perpendicular mean free paths, it is clear that NLGC-E and NLGC-S agree well, which can also be seen for the simulations shown in the following figures. We can also see that the disagreement between FLRW and all the simulation results in this paper for perpendicular diffusion is significant, so we do not show the FLRW results in the rest of the figures.

Yet another series of simulation results is shown in Figure 3 for perpendicular (*top*) and parallel (*bottom*) mean free paths as a function of $E_{\rm slab}/E_{\rm tot}$ with $r_{\rm L}/\lambda_c = 0.048$ and $b/B_0 = 1$. The bottom panel shows that NLGC-E agrees well with simulations for parallel mean free paths over the entire range of $E_{\rm slab}/E_{\rm tot}$ from pure slab to pure 2D turbulence, while QLT generally does not agree with simulations unless there is nearly pure slab turbulence.

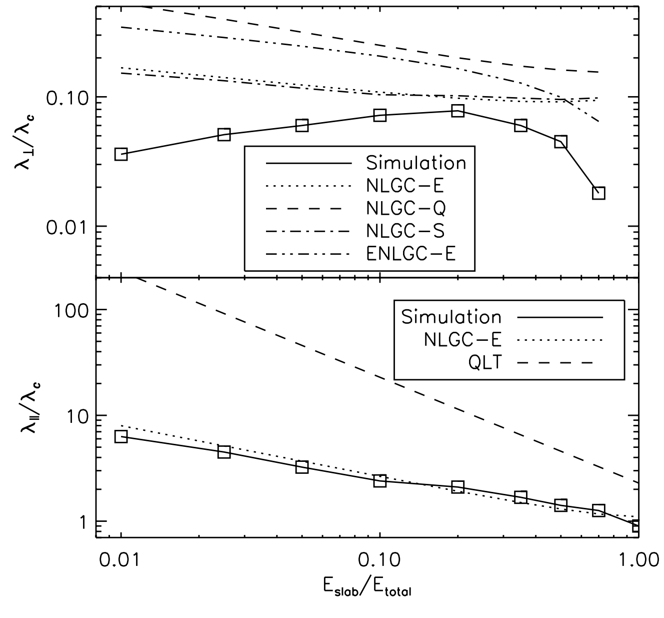

FIG. 3.—Perpendicular (*top*) and parallel (*bottom*) mean free paths as a function of $E_{\rm slab}/E_{\rm tot}$, with $r_{\rm L}/\lambda_c = 0.048$ and $b/B_0 = 1$.

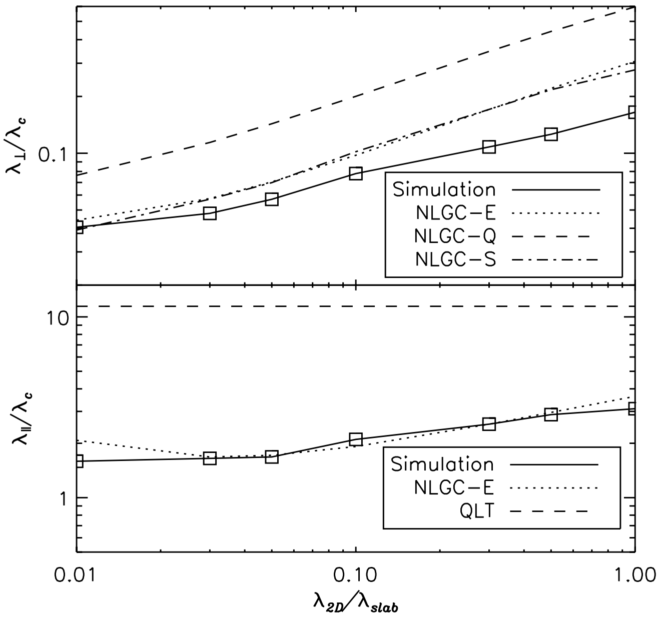

FIG. 4.—Perpendicular (*top*) and parallel (*bottom*) mean free paths as a function of $\lambda_{\rm 2D}/\lambda_{\rm slab}$, with $r_{\rm L}/\lambda_c = 0.048$, $E_{\rm slab}/E_{\rm tot} = 0.2$, $b/B_0 = 1$, and $\tilde{\lambda}/\lambda_{\rm slab}$ varying from 0.44 to 3.

The top panel of Figure 3 shows that for perpendicular mean free paths NLGC-E agrees well with simulations except in nearly pure 2D turbulence or in turbulence with a larger slab component in energy. However, NLGC-Q is much worse than NLGC-E when QLT does not agree with simulations for parallel mean free paths. Note that for the simulation results for particles in nearly pure 2D turbulence, we show the parallel mean free paths in the bottom panel but do not show the perpendicular mean free paths, because particles transport subdiffusively when turbulence lacks a strong 3D structure (Urch 1977; Kóta & Jokipii 2000; Qin et al. 2002a).

As a reference, in Figure 3 we also show the results from ENLGC-E, the combination of the modified NLGC (ENLGC; Shalchi 2006) and NLPA. Based on NLGC, if we assume that only the 2D component of turbulence contributes to the perpendicular diffusion mean free paths with a large timescale and that the constant $a = 1$, ENLGC is obtained. In Figure 3 (*top*), the dot-dot-dashed line indicates the perpendicular mean free paths from ENLGC-E. From the comparison of NLGC-E and ENLGC-E, we have the following results. When $0.5 < E_{\rm slab}/E_{\rm tot} \lesssim 0.7$, ENLGC-E agrees somewhat better with simulations for perpendicular mean free paths than NLGC-E does, but neither of the theories agrees well with simulations. On the other hand, when $E_{\rm slab}/E_{\rm tot} < 0.5$, ENLGC-E agrees worse with simulations for perpendicular mean free paths than NLGC-E does. For parallel mean free paths, NLGC-E and ENLGC-E have similar results, so in Figure 3 (*bottom*) we only show the results from NLGC-E.

In order to study the effect of the turbulent correlation scale of the 2D component on diffusion coefficients, we show an additional series of simulation results in Figure 4 for perpendicular (*top*) and parallel (*bottom*) mean free paths as a function of $\lambda_{\rm 2D}/\lambda_{\rm slab}$ with $r_{\rm L}/\lambda_c = 0.048$, $E_{\rm slab}/E_{\rm tot} = 0.2$, $b/B_0 = 1$, and $\tilde{\lambda}/\lambda_{\rm slab}$ varying from 0.44 to 3. The bottom panel shows that NLGC-E agrees well with simulations for parallel mean free paths as $\lambda_{\rm 2D}/\lambda_{\rm slab}$ increases from 0.01 to 1, while QLT does not agree with simulations. Figure 4 (*top*) shows that for perpendicular mean free paths NLGC-E agrees much better with simulations than NLGC-Q does. In addition, the agreement between NLGC-E and simulations becomes worse with the large correlation scale of 2D turbulence

($\lambda_{2D}/\lambda_{slab} \gtrsim 0.5$) when the turbulence's three dimensional (3D) structure becomes weaker.

4. SUMMARY AND DISCUSSION

In this paper, starting from the method used to calculate the pitch-angle diffusion coefficient by Jokipii (1966), we develop a theory of the parallel diffusion of charged particles with nonlinear and dynamical effects. Similar to the assumption in Matthaeus et al. (2003) that particle gyrocenters following magnetic field lines leads to parallel velocity decorrelation, we assume perpendicular velocity decorrelation because of the particle's parallel scattering and the direct contribution of turbulence. With a series of additional approximations used in Matthaeus et al. (2003), such as Corrsin's independence hypothesis, uncorrelated axisymmetric Gaussian distributions for trajectory components, and the diffusive distribution of displacements, the nonlinear parallel diffusion theory (NLPA) is obtained with the perpendicular diffusion coefficient included explicitly. With the combination of NLGC and NLPA we get an extended nonlinear guiding center theory, NLGC-E.

From a comparison of simulations and theoretical results we arrive at the following conclusions. First, FLRW does not generally agree with simulations for perpendicular mean free paths. Second, QLT agrees with simulations when nonlinear effects are not important, i.e., when turbulence is nearly pure slab, or when particles have relatively large rigidity and turbulence is weak. Third, NLGC-E generally agrees well with simulations for parallel mean free paths. Fourth, NLGC-E agrees well with simulations for perpendicular mean free paths unless there is turbulence with a nearly pure 2D component or a slab component that is stronger than the 2D component. The reason that NLGC-E is not valid in nearly pure 2D turbulence for perpendicular mean free paths might be that the 2D component is so strong that field lines are trapped by the 2D island and the perpendicular field line diffusion is suppressed; therefore, the perpendicular diffusion of particles is suppressed (Chuychai et al. 2005). However, the NLGC-E does not take this effect into account. Furthermore, we assume that the reason NLGC-E is not valid in turbulence with more slab component energy or with a large correlation scale of the 2D component is that, under these conditions, the turbulence has less 3D structure, the similarity of nearby field lines is significant, and the particles' transport is in a transit regime between true diffusion and subdiffusion, so the measured perpendicular mean free paths decrease dramatically (Urch 1977; Kóta & Jokipii 2000; Qin et al. 2002a, 2002b). However, in the derivation of NLGC-E true diffusion is assumed. Fifth, NLGC with parallel mean free paths from simulation results as input, NLGC-S, agrees with NLGC-E for perpendicular mean free paths well. Sixth, NLGC with parallel mean free paths from QLT as input, NLGC-Q, agrees with simulations for perpendicular mean free paths only when QLT agrees with simulations well. Seventh, ENLGC-E, the combination of ENLGC (modified NLGC; Shalchi 2006) and NLPA, generally gives worse agreement with simulations for perpendicular mean free paths than NLGC-E does unless the slab component of turbulence is stronger than the 2D one. We think the reason is that in the composite model of turbulence with a strong transverse structure, the slab component of turbulence will still contribute to the perpendicular diffusion on a large timescale. Shalchi et al. (2004) also show that the WNLT agrees much better with simulations for parallel and perpendicular mean free paths than QLT or FLRW. However, NLGC-E has a much simpler mathematical form and is much more computationally tractable, and in practice, we could use NLGC-E for theoretical studies of the diffusion of particles.

Both of our numerical and theoretical results from NLGC-E show that the 2D component of turbulence contributes to the mean free paths of energetic particles in strong turbulence or when particles' energies are relatively low, which is in contrast to the QLT assumptions. Thus, the theoretical explanation of the problem of the solar energetic particles' "too small" mean free paths (Palmer 1982; Bieber et al. 1994) needs to be revisited (Qin et al. 2006). However, in this work we do not compare NLGC-E results with observations from spacecraft, since the turbulence spectrum we use here does not include dissipation range and dynamical effects, as in the solar wind. In future work, a realistic turbulence spectrum will be used so that a comparison of theoretical results with observations can be made (Bieber et al. 1994; Shalchi et al. 2006). Furthermore, it is possible that the dynamical effects may help to recover perpendicular diffusion in turbulence with a nearly pure 2D mode or with a larger slab component than a 2D component in energy. Thus, NLGC-E might become valid under these conditions too. We hope this new theory, NLGC-E, can help us understand some of the observational difficulties in a realistic turbulence spectrum.

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