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Particle-in-cell experiments examine electron diffusion by whistler-mode waves: 1. Benchmarking with a cold plasma

O. Allanson¹, C. E. J. Watt¹, H. Ratcliffe², N. P. Meredith³, H. J. Allison^{3,4}, S. N. Bentley¹, T. Bloch¹ & S. A. Glauert³

¹Space & Atmospheric Electricity Group; Department of Meteorology; University of Reading; Reading; UK ²Centre for Fusion, Space and Astrophysics; Department of Physics; University of Warwick; Coventry; UK ³British Antarctic Survey, Natural Environment Research Council, Cambridge; UK ⁴Helmholtz Centre Potsdam - GFZ German Research Centre for Geosciences: Potsdam; Germany

Key Points:

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10	•	Particle-in-cell numerical experiments track electron pitch-angle diffusion due to
11		whistler-mode wave-particle interactions
12	•	Our novel approach directly extracts diffusive characteristics across all energy and
13		pitch angle space
14	•	After an initial transient phase we observe a normal diffusive response that is con-
15		sistent with quasilinear theory

 $Corresponding \ author: \ Oliver \ Allanson, \verb"o.allanson@reading.ac.uk"$

16 Abstract

Using a particle-in-cell code, we study the diffusive response of electrons due to wave-17 particle interactions with whistler-mode waves. The relatively simple configuration of 18 field-aligned waves in a cold plasma is used in order to benchmark our novel method, 19 and to compare with previous works that used a different modelling technique. In this 20 boundary-value problem, incoherent whistler-mode waves are excited at the domain bound-21 ary, and then propagate through the ambient plasma. Electron diffusion characteristics are directly extracted from particle data across all available energy and pitch-angle space. 23 The 'nature' of the diffusive response is itself a function of energy and pitch-angle, such 24 that the rate of diffusion is not always constant in time. However, after an initial transient 25 phase, the rate of diffusion tends to a constant, in a manner that is consistent with the as-26 sumptions of quasilinear diffusion theory. This work establishes a framework for future 27 investigations on the nature of diffusion due to whistler-mode wave-particle interactions, 28 using particle-in-cell numerical codes with driven waves as boundary value problems. 29

³⁰ Plain language summary

'Whistler-mode' plasma waves interact with electrons in the Earth's outer radiation belts. 31 This wave-particle interaction plays a significant role in both electron acceleration, and 32 in the loss of electrons to the atmosphere via 'pitch angle scattering'. Such processes are 33 typically modelled using numerical diffusion codes, with electron diffusion coefficients 34 that characterize the nature and the strength of the wave-particle interaction. These dif-35 fusion coefficients are calculated using a mixture of long-established theory and input 36 parameters taken from data and/or empirical models. We present a novel method for the 37 direct extraction of characteristics of the electron diffusion from particle-in-cell numerical 38 experiments. Our results demonstrate that the rate of diffusion can be time-dependent at 39 early times, but then tends to constant values in a manner that is consistent with quasilin-40 ear theory. 41

42 **1** Introduction

Wave-particle interactions are a key source of variability in the outer radiation belt 43 (e.g. Horne et al. [2005a]; Thorne [2010]; Reeves et al. [2013]). Decades of research into 44 the behaviour of high-energy electrons in Earth's magnetosphere has determined that wave-45 particle interactions over a range of different frequencies can diffuse the particles in phase-46 space, leading to energisation and loss of high-energy particles that could explain the vari-47 ability of the belts (e.g. Fälthammar [1965]; Hudson et al. [2000]; Thorne et al. [2013]). 48 Whistler-mode waves are electromagnetic waves that propagate below the electron gyrofrequency (e.g. see Artemyev et al. [2016a]) and can interact with electrons across a wide 50 range of energies (e.g. Horne et al. [2005b]; Thorne et al. [2010]). Whistler-mode waves 51 take a range of different forms: narrowband transmitter waves are artificially-generated at 52 Earth's surface by high-power radio transmitters (e.g. Zhang et al. [2018b]; Meredith et al. 53 [2019]); lightning-generated whistlers are generated by lightning and propagate upwards 54 through the ionosphere into the magnetosphere (e.g. Němec et al. [2010]); whistler-mode 55 chorus is naturally generated by plasma instabilities within the Earth's magnetosphere (e.g. 56 Omura et al. [2007]; Meredith et al. [2009]; Chen et al. [2017]; Gao et al. [2017]); inco-57 herent plasmaspheric hiss [Bortnik et al., 2008a; Chen et al., 2012, 2014] has a number of 58 established source mechanisms (e.g. see Meredith et al. [2018] for a discussion of these). 59

Current approaches to modelling the effect of wave-particle interactions in the outer radiation belt most typically use the quasilinear theory (QLT) [*Kennel and Engelmann*, 1966; *Lerche*, 1968; *Lyons*, 1974]. This formalism describes wave-particle interactions as diffusive processes in the plasma, flattening out gradients and moving electrons to different energies and/or different pitch-angles. The exact form of the equations used in the model depends on the characterization of the wave-particle interactions that are responsible for

the diffusive behaviour, and this characterization is provided by the diffusion coefficients. 66 The analytic form of diffusion coefficients are derived using QLT, and then implemented 67 in diffusion codes by using models of wave and plasma parameters (e.g. see Glauert et al. [2014]). Formally, the application of QLT to wave-particle interactions places a number 69 of restrictions on the plasma waves considered, typically considered to be that the waves 70 are incoherent and of low amplitude [Stix, 1992; Treumann and Baumjohann, 2001]. How-71 ever, observations of whistler-mode waves in the inner magnetosphere (e.g. Cattell et al. 72 [2008]; Cully et al. [2008]; Breneman et al. [2011]; Wilson III et al. [2011]; Kellogg et al. 73 [2011]; Gao et al. [2016]) have revealed that wave amplitudes can be orders of magnitude 74 larger than previously thought. Furthermore, it is evident from observations that certain 75 whistler-modes possess structure and/or coherency in frequency space, e.g. the rising and 76 falling tones of chorus emissions, and the nearly monochromatic signals of transmitter 77 waves. Hence there is strong evidence that motivates from-first-principles investigations of 78 whistler-mode wave-particle interactions in the outer radiation belt. 79

There are a large number of theoretical calculations and numerical experiments rele-80 vant to the work presented in this paper and so it is not possible to discuss every one (e.g. 81 a non-exhaustive list of such works on whistler-mode wave-particle interactions includes 82 Albert [2001, 2002]; Omura et al. [2007]; Bortnik et al. [2008b]; Albert [2010]; Tao and 83 Bortnik [2010]; Tao et al. [2011, 2012a,b, 2013]; Camporeale and Zimbardo [2015]; Cam-84 poreale [2015]; Mourenas et al. [2018]; Silva et al. [2018]). Instead, we focus on some of the works that - either with test-particle or particle-in-cell (PiC) codes - analyzed the sta-86 tistical/diffusive response of the plasma, by directly extracting particle data. Bortnik et al. [2008a] used test-particle experiments in a dipolar magnetic field to model the effect of 88 large amplitude and oblique monochromatic chorus waves on the particle response. It was found that the wave-particle interaction changed qualitatively from that of diffusion be-90 yond a certain amplitude, in which case a nonlinear approach was found necessary. The nature of the nonlinear behaviour observed (diffusive, phase bunching or phase-trapping) 92 was found to correlate with those predicted in Albert [2002] for different wave and plasma 93 regimes. The nonlinear behaviour also varies according to a inhomogeneity parameter 94 that indicates whether or not quasi-linear theory is applicable in the narrowband limit 95 (discussed in e.g. Bortnik et al. [2008a]; Omura et al.; Tao and Bortnik [2010]; Tao et al. [2012a]). Tao et al. [2011] used a test-particle code to study the response of electrons to a 97 uniform spectrum of incoherent, broadband and small amplitude waves in a homogeneous 98 background field, but specifically targeted electron populations predicted to be in reso-99 nance. They found that the electron response was indeed stochastic and in excellent agree-100 ment with QLT. Tao et al. [2012a] performed test-particle simulations for field-aligned 101 waves in a simplified dipole field model (no curvature), and found (also for resonant par-102 ticles only) that the bounce-averaged quasi-linear diffusion coefficients became invalid as 103 the wave amplitude surpassed given thresholds. Specifically, they found this threshold to be $|B_{w,rms}^2/B_0^2| \ge 2 \times 10^{-7}$ for 10keV electrons, and $|B_{w,rms}^2/B_0^2| \ge 7 \times 10^{-6}$ for 1MeV 105 electrons, where waves have root-mean-squared amplitudes of magnitude $B_{w,rms}$ in a back-106 ground field B₀. Camporeale and Zimbardo [2015] used self-consistent kinetic simulations 107 to investigate diffusion during the linear growth phase and saturation of anisotropy-driven 108 instabilities that self-consistently generate whistler-mode waves. They found evidence of 109 nonlinear and time-dependent effects, with enhanced pitch angle diffusion during the linear 110 growth phase. In a similar experiment, Camporeale [2015] investigated diffusion due to 111 the self-consistently generated lower-band chorus waves, and compared to the predictions 112 given by a QLT diffusion code. Specifically, they found significant mismatch in regions 113 of phase-space for which the resonance condition is not satisfied, and called for nonlin-114 ear theories in order to capture non-resonant interactions. We also note that there is re-115 cent theoretical work based upon using kinetic equations used to describe the evolution of 116 the particle energy distribution due to nonlinear wave-particle interactions Artemyev et al. 117 [2016b, 2017, 2018]; Mourenas et al. [2018]; Vainchtein et al. [2018], and for which one 118 of the main aims is "to incorporate nonlinear effects of intense, short-duration chorus wave 119 packets into global (quasilinear) diffusion models" (Quoted from presentation, J. Bortnik, 120

ISSS-13, September 6-14 2018, UCLA). We note that the standard quasilinear diffusion
 theory sometimes captures observed diffusive properties surprisingly well, even in circum stances for which the assumptions of the theory are formally invalid (e.g. see a discussion
 in *Zhang et al.* [2018a]).

The standard test-particle approach to modelling wave-particle interactions presents 125 both advantages and disadvantages. Test-particle codes are (relatively) cheap to run nu-126 merically and enable one to implement wave modes of exactly the desired form. However, 127 wave-particle interactions are a fundamentally kinetic physics process, and test-particle 128 codes do not include all of the self-consistent interactions between particles and wave 129 fields. Particle-in-cell experiments enable users to model these self-consistent interactions, 130 and in principle allow a greater range of kinetic-physics diagnostics (e.g. the distribution 131 function). Indeed, it has recently been shown that using the two different approaches to 132 study diffusion due to whistler mode wave-particle interactions can yield markedly differ-133 ent results [Camporeale and Zimbardo, 2015; Camporeale, 2015]. Here, we use a mix-134 ture of both the test-particle and particle-in-cell approaches. We exploit the self-consistent 135 PiC interaction to model the waves as they propagate through the plasma, instead of pre-136 scribing fixed-characteristic waves as in a test-particle approach. The inclusion of sub 137 electron-scale physics in the interaction between the background plasma and the propa-138 gating waves will allow the whistler-mode waves to fluctuate on sub-electron spatial and 139 temporal scales. In the simulation, we release a very large number of tracer ('test') particles in order to extract characteristics of the pitch-angle diffusion for electrons across all 1/1 available energies and pitch-angles. These tracer particles contribute no 'moments' to the 142 particle-in-cell algorithm, and respond to the electromagnetic fields in the same way as the 143 methods in Tao et al. [2011], for example. In using a combination of both self-consistent particle-in-cell and test-particle methods, we should expect to see both similarities and 145 differences in the results obtained when compared to Tao et al. [2011]. 146

In particular, our intent in this first paper of a series is to study the nature of the dif-147 fusion when the waves propagate in one dimension along the background magnetic field in 148 a cold, homogeneous plasma. This initial 'benchmarking' scenario showcases our method 149 and indicates similarities to and differences from the test-particle results reported in previ-150 ous work (e.g. Tao et al. [2011]). Future papers in this series will compare the strength of 151 the effective diffusion coefficients extracted from the PiC experiment with the size of the 152 analytic quasilinear diffusion coefficient across all of pitch-angle/energy space, and will re-153 peat the numerical experiment for whistler-mode wave propagation through a plasma with 154 the fractional warm components that can be found in Earth's inner magnetosphere. 155

This paper is organized as follows. In Section 2 we describe the philosophy and setup of the numerical experiments, including the numerical scheme. In particular we discuss the wave excitation mechanism and the properties of the electromagnetic waves within the domain. Diffusion theory as is applicable to the outer radiation belt is discussed in Section 3. Results from the numerical experiments, including the diffusive plasma response are discussed in Section 4. In Section 5 we discuss our results in more detail and put the results in context. Section 6 contains a summary, including motivation for future investigations that will build upon the results reported here.

¹⁶⁴ **2** Outline of experiments

Radiation belt diffusion coefficients are fundamentally a function of both the plasma and wave parameters, i.e., the plasma density, background magnetic field, wave strength and wave spectral form. As a result, the direct evaluation of a diffusion coefficient relies on both the plasma and wave characteristics being quasi-static for the time over which they are calculated [*Schulz and Lanzerotti*, 1974]. Therefore we consider a boundary value problem, in which we perturb the left-hand boundary with a given specific wave spectrum, which then excites electromagnetic waves that propagate throughout the experimental do-

main. The perturbation mechanism is applied at all times, and this enables us to study 172 the interaction for a wave spectrum that is quasi-static in amplitude (root-mean-squared) 173 and spectral form. However, the wave spectrum does exhibit some small-scale spatial and 174 temporal fluctuations in response to self-consistent interactions with the background cold 175 plasma. This approach is in contrast to an initial value problem, in which one might study 176 the self-consistent generation mechanism and subsequent evolution of waves in an initially 177 unstable plasma, and for which the wave spectra is more variable in time (e.g. Katoh and Omura [2006]; Omura et al.; Hikishima et al. [2009]; Omura et al. [2009]; Omidi et al. 179 [2010, 2011]; Katoh and Omura [2013]; Camporeale [2015]; Camporeale and Zimbardo 180 [2015]; Silva et al. [2017]; Ratcliffe and Watt [2017]; Katoh et al. [2018]). In Tao et al. 181 [2011], a relativistic test-particle code was used to study the diffusive plasma response 182 due to wave-particle interactions of driven, broadband and incoherent waves waves with 183 magnetospheric plasma populations appropriate for the outer radiation belt at 6 Earth radii 184 $(r \sim 6R_{\rm E})$. Our experimental parameters are chosen in order to resemble those in *Tao et al.* 185 [2011] as far as possible. 186

187

2.1 Numerical experiment design

Wave-particle interactions are a fundamentally kinetic plasma physics process, since 188 their efficiency explicitly depends on particle-scale physics, as statistically described by the 189 particle distribution function. We use the EPOCH PiC code [Arber et al., 2015], which is 190 described in more detail in Appendix A. Essentially, the numerical experiments involve exciting waves of specified frequencies from an "antenna" at one of the spatial boundaries 192 of the simulation domain. Electromagnetic waves then propagate through the domain, self-193 consistently interacting with the cold plasma component of the plasma interior. We also 194 release a large number of non-interacting 'tracer' particles that are used to monitor the 195 diffusion in different regions of pitch-angle/energy space. These particles contribute no 196 moments to the PiC algorithm. The tracer particles act as 'labels' in phase-space such 197 that their collective diffusive response can be categorized as a function of pitch angle and 198 energy. 199

As a first step, we restrict the experimental domain to one field-aligned dimension 200 (x). On the compressed dayside magnetosphere near the magnetic equator, uniform fields 201 and field-aligned wave propagation is a reasonable approximation [Tsurutani and Smith, 202 1977]. We do so in order to fully understand the most idealized example of this wave-203 particle interaction, before introducing new effects in isolation (e.g. oblique wave propagation, field inhomogeneities, and modifications to the wave spectra). EPOCH uses a Carte-205 sian grid, which in 1-D means that all quantities may vary in the x direction only. We set 206 an ambient magnetic field, $\mathbf{B}_0 = (B_{x0}, 0, 0)$, with $B_{x0} = 140$ nT, and so refer to x as parallel 207 (||), y and z as perpendicular (\perp).

We model a uniform cold 'background' plasma with number density, $n_{\rm b} = 10^7 {\rm m}^{-3}$. 209 For this cold background plasma, and ambient magnetic field, the ratio of electron plasma 210 frequency to non-relativistic gyrofrequency is given by $\omega_{\rm pe}/|\omega_{\rm ce}| \approx 7.2$, for $\omega_{\rm pe} = \sqrt{ne^2/(m_e\epsilon_0)}$, 211 and $\omega_{ce} = q_e B_0/m_e < 0$ in the uniform background field. We describe the ambient 212 plasma by using cold ion and electron populations with initial spatially uniform number 213 density of $n_{\rm b}$ and isotropic temperature of 0.1eV. These choices are motivated by our de-214 sire to emulate, as far as possible, the scenario of *Tao et al.* [2011]. In a warm plasma, or 215 plasma with fractional warm components, the wave amplitudes would be expected to al-216 tered by the presence of the warm component. If the plasma is isotropic, then the waves will damp/reduce their amplitude, and if the plasma has positive anisotropy then the waves 218 may grow in amplitude through the appropriate kinetic wave-particle interaction. In this 219 numerical experiment, we choose a cold plasma environment in order to ensure that waves 220 entering the domain do not change amplitude significantly as they propagate through the 221 plasma. 222

The real world run time for the experiment is $T = 575t_{ce} \approx 0.15s$, for $t_{ce} = 1/f_{ce}$ 223 with $f_{ce} = |\omega_{ce}|/(2\pi) \approx 3919$ Hz. We use 500 particles-per-cell per species; physical 224 values of proton-electron mass ratio, $m_i/m_e = 1836.2$; and the speed of light is set to its 225 real value $c \approx 3 \times 10^8 \text{ms}^{-1}$. Periodic boundary conditions are chosen for the particles, 226 whereas electromagnetic waves have open boundary conditions (the electromagnetic field 227 boundary condition works by allowing outflowing characteristics to propagate through the 228 boundary with as little reflection as possible). The domain length, $L = 40\lambda_{lc}$, is set to be 40 times the estimated wavelength inside the domain, $\lambda_{lc} = c/(\eta f_{lc})$, of the lowest 230 frequency wave emitted by the antenna, $\omega_{lc} = 2\pi f_{lc}$. The refractive index is a function of 231 frequency, $\eta = \eta(\omega)$, and is determined by the cold plasma dispersion relation [Stix, 1992; 232 Omura et al., 2007], 233

$$\eta^{2} = \frac{c^{2}k^{2}}{\omega^{2}} = 1 + \frac{\omega_{\rm pe}^{2}/\omega^{2}}{|\omega_{\rm ce}|/\omega - 1}.$$
(1)

We use 3587 cells in the *x*-direction, with grid spacing $\Delta x \approx 235$ m, such that $\Delta x/(c/|\omega_{ce}|) \approx 0.02$. The Debye radius, $\lambda_D = \sqrt{\epsilon_0 k_B T_e/(n_b q_e^2)} \approx 2.35$ m is not resolved by Δx , and we have $\Delta x/\lambda_D = 100$. It is well-known that particle-in-cell experiments are in principle vulnerable to the self-heating phenomenon, and that this can be mitigated by choosing $\Delta x \approx \lambda_D$ in explicit codes. However, it is absolutely possible to perform valid and physically meaningful particle-in-cell numerical experiments with a value of Δx that does not resolve the Debye radius (e.g. see a discussion in [*Arber et al.*, 2015]). In particular, if one can demonstrate that for a particular choice of Δx :

242 243 1. all necessary physical scales have been resolved that are most important for the phenomenon of interest,

2. the self-heating is limited to a reasonable level,

then it is entirely justifiable to have $\Delta x > \lambda_D$. It is not uncommon to use such values, e.g. two examples of works that discussed results of explicit PiC experiments using a spatial resolution $\Delta \gg \lambda_D$ include: (i) *Ratcliffe and Watt* [2017] with $\Delta/\lambda_D \approx 139$, in which the '0.5 cyclotron frequency gap' in magnetospheric whistler-mode waves was selfconsistently generated; (ii) *Tsiklauri* [2016] with $\Delta/\lambda_D \approx 200 - 270$, for the study of electron plasma wakefield acceleration.

We justify point 1. for our experiment as follows. Our chosen value of Δx resolves 251 the electron inertial length according to $\Delta x/d_e \approx 0.07$, for $d_e = c/\omega_{\rm pe} \approx 1680$ m, and 252 therefore resolves the fundamental scale of electron kinetic physics. Furthermore, it re-253 solves the shortest wavelength of the whistler-mode wave spectrum that is important for 254 the wave-particle dynamics in this study, $\Delta x/\lambda_{uc} \approx 0.009$, for $\lambda_{uc} = c/(\eta f_{uc})$ and η de-255 termined by equation (1). Therefore, our chosen grid discretization resolves electron scale 256 kinetic physics, and in particular the spatial scales necessary for electron wave-particle 257 interactions with the driven whistler-mode waves. 258

We justify point 2. for our experiment as follows. The classic constraint $\Delta x \approx \lambda_D$ 260 [Langdon, 1970] relates to the case where particle forces are assigned to 'nearest-neighbour' 261 grid points, and for which the underlying scheme is momentum-conserving. EPOCH is a 262 charge-conserving code, with capability to use higher-order shape functions: such weight-263 ing schemes suffer from a less catastrophic form of self-heating, and generally with a low 264 265 growth rate. In this work we triangular shape functions (a 3 point stencil, 2 cells wide). A discussion of stability and self-heating in EPOCH, with reference to shape-functions, 266 is given in Section 5 of Arber et al. [2015]. The EPOCH code also provides one further 267 method to limit the noise in the PiC simulation, and which we use in this work: ' δF 268 mode' (as detailed in Appendix A). In figure 1 we present an analysis of the temporal 269 evolution of the electromagnetic and particle energies within the experimental domain, with special consideration of the electromagnetic energy flux through the boundaries. The 271 experiment utilizes periodic boundary conditions for the particles. However, there is a 272 constant input of electromagnetic energy into the domain via the wave excitation method, 273

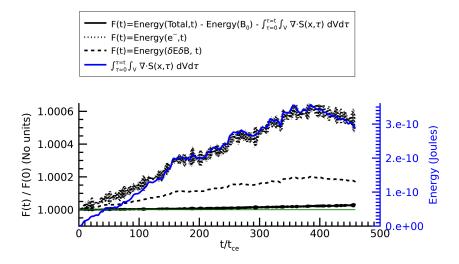


Figure 1. Evolution of the energy budget within the experiment.

and outgoing electromagnetic wave energy is permitted to flow out of the experimen tal domain. Therefore the total energy will not be conserved, but the following quantity

should be conserved,

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$$E_{KE}(t) + E_{EM,\text{domain}}(t) - E_{S,\text{boundary}}(t) = \text{const.}$$
(2)

The three terms on the left-hand-side represent, respectively: (a) the kinetic energy of all ions and electrons; (b) the total electromagnetic energy within the domain; (c) the timeintegrated net electromagnetic power that has entered the domain up to time t,

$$E_{S,\text{boundary}}(t) := \int_{\tau=0}^{\tau=t} \int_{V} \nabla \cdot \mathbf{S}(x,t) dV d\tau$$

for S the Poynting vector. This time-integrated power (energy) represents the only means 280 by which the total energy budget within the experimental domain should change. In fig-281 ure 1 we plot the normalized evolution of the quantity in equation (2) minus the energy 282 associated with the time-independent and homogeneous background magnetic field (with 283 a solid black line). Stability of the numerical code required that this quantity should not 284 diverge significantly from unity. Figure 1 shows conservation of the net simulation energy 285 to better than 0.1%, confirming that self heating is minimal. In figure 1 we also plot the 286 evolution of: total electron energy (black dots); total energy associated with electromagnetic fluctuations within the domain (black dashes); and the time-integrated electromag-288 netic power that has entered the domain up to time t (solid blue line). We see that the to-289 tal electron energy clearly tracks the injected wave energy and the total energy associated 290 with the EM fluctuations. 291

2.2 Wave spectra

We excite the plasma at the left-hand boundary (x = 0) using EPOCH's using EPOCH's driven boundary option, (called 'laser' after its most common use), such that the perturbations propagate in the positive-*x* direction. For each given specified frequency, this boundary condition simply perturbs the domain with a (sinusoidal) time-varying electromagnetic field. We superpose a collection of different perturbations, with the intent to reproduce the spectrum used in *Tao et al.* [2011]. We specify a discrete sum of $N_{wave} =$ 100 individual right-hand polarized electric field perturbations. Each one of the 100 modes is composed of 2 linearly polarized components, with wave fields that oscillate in the y and z directions respectively,

$$\mathbf{E}_{\text{wave}}(x,t) = \sum_{i=1}^{N_{\text{wave}}} \mathbf{E}_{\text{wave},i}(x,t) = \sum_{i=1}^{N_{\text{wave}}} \mathbf{E}_{\text{wave},y,i}(x,t) + \mathbf{E}_{\text{wave},z,i}(x,t),$$

Each pair of linearly polarized waves, ($\mathbf{E}_{wave, y, i}$, $\mathbf{E}_{wave, z, i}$), has the appropriate phase shift between themselves such as is required for right-handed polarization [*Stix*, 1992]. Each mode, $\mathbf{E}_{wave, i}$, also has a random phase, and a frequency that is uniformly selected from the range

$$f_{\rm lc} = 0.2 f_{\rm ce} \le f \le 0.4 f_{\rm ce} = f_{\rm uc}.$$

Full details on how to prescribe such a spectrum are given in *Tao et al.* [2011], and we include the text file that prescribes the perturbation as supplementary information (S2).

Given these user inputs for the electric field perturbations, the Maxwell solver in 308 EPOCH generates self-consistent magnetic field perturbations ($\mathbf{B}_{wave,i}$) in accordance with 309 Maxwell's equations. We choose the magnitude of the electric field perturbations so that 310 they are (in principle) consistent with corresponding magnetic field perturbations of 1pT 311 in a vacuum ($|\mathbf{E}_{wave,i}| = c|\mathbf{B}_{wave,i}|$, and such that $|\mathbf{B}_{wave,i}| = 1$ pT). We note here that 312 our perturbation method is intended to excite the whistler-mode wave branch of the cold 313 plasma dispersion relation [Stix, 1992], since a cold plasma can support whistler-mode wave propagation when excited at these frequencies. A 'fully self-consistent' wave driv-315 ing technique would also necessitate the self-consistent perturbations of other oscillat-316 ing macroscopic quantities, e.g. polarization currents. However, that approach is much 317 more complicated and beyond the scope of this work. Regardless of the specific excitation 318 technique, and as will be shown, we are able to excite the electromagnetic component of 319 whistler-mode waves within the interior of the plasma. Once excited, these components 320 then propagate and continue to be supported by (and interact self-consistently with) the 321 background cold-plasma. 322

Sudden electromagnetic perturbations can often cause undesired 'shock' effects in 323 a simulated plasma at the moment the perturbation is 'switched on'. In order to eliminate 324 any such effects, we apply a linear envelope to the wave profile, so that for $t < 2/f_{\rm lc}$, 325 the wave profile has amplitude scaled by 1/t. This prevents any shock effects from oc-326 curring. It takes approximately $t_{cross} = 115t_{ce}$ for the wave profile to cross the experi-327 mental domain, from left to right. All wave and particle analysis in this paper pertains to 328 times after this time, $t > t_{cross}$. Therefore we analyze only over times during which the 329 entire experimental domain is interacting with the propagating waves. Since the run time 330 of the experiment is $T = 575t_{ce}$, we analyze wave-particle interactions for a total time of $T - t_{\rm cross} = 460t_{ce}$. This corresponds to ≈ 92 wave periods for waves with frequency f_{lc} , 332 and ≈ 184 wave periods for waves with frequency f_{uc} . For completeness, we plot the B_y 333 (red) and E_{y} (blue) components of the electromagnetic fields as a function of x in figure 334 2. This figure includes the waveform at: (a) $28t_{ce}$, soon after the completion of the linear envelope scaling of the excitation; (b) $143t_{ce}$, soon after the wave has crossed the domain; 336 (c) $280t_{ce}$, roughly half-way through the numerical experiment; (d) $561t_{ce}$, close to the end 337 of the experiment. 338

341 One important difference between our work and that of *Tao et al.* [2011], is that the wave-spectrum excited by the antenna on the left-hand boundary is not exactly reproduced 342 within the domain. Since we use a fully kinetic numerical code, the driven waves interact 343 self-consistently with the background plasma populations via Maxwell's equations, where 344 the current density is derived directly from the flux of different species' super-particle 345 populations. The background plasma super-particle populations evolve in a self-consistent manner via the (relativistic) Lorentz force equation. This is all at the cost of higher com-347 putational expense, as compared to a test-particle simulation. However, we consider the 348 freedom to have fully self-consistent wave-particle interactions to be a benefit of using the 349

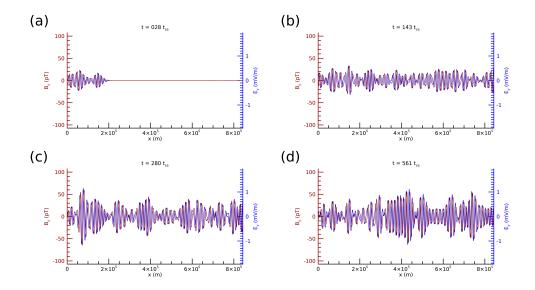


Figure 2. The B_y (red) and E_y (blue) components of the electromagnetic fields as a function of x at: (a) 28 t_{ce} ; (b) 143 t_{ce} ; (c) 280 t_{ce} ; (d) 561 t_{ce} .

PiC approach for this study, and therefore the benefits of using fully self-consistent PiC compensate for the added computational cost.

Figure 3 shows the 'one-sided' Fourier amplitude spectrum of the B_{y} (red) and E_{y} 359 components (blue) of the waves, averaged over all space (within the PiC domain) and 360 time during the wave-particle interaction ($460t_{ce}$, i.e. $t > t_{cross}$). The Fourier amplitude 361 is defined such that a single wave ~ $A \sin(kx \pm wt)$ will have amplitude |A|. The vertical 362 black lines mark the lower and upper bounds of the driven wave spectrum ($f_{lc} = 0.2 f_{ce}$ 363 and $f_{uc} = 0.4 f_{ce}$ respectively), whilst the vertical green line marks the electron gyro-364 frequency f_{ce} . The horizontal black line marks a continuous version of the B_{y} spectrum 365 employed by *Tao et al.* [2011]. The waves clearly show dominant power within the re-366 quired frequency domain. However, there is some amplification as compared to the uni-367 form 1pT spectrum as used by Tao et al. [2011], and we observe non-zero amplitudes 368 outside the driven frequency domain (f_{lc}, f_{uc}) . We observe a root-mean-square wave am-369 plitude of $B_{\rm w,rms} \approx 25 \rm pT$ in our experiment, slightly higher than the value of 10pT that 370 Tao et al. [2011] use. This difference is, in reality, a small one, and a result of the diffi-371 culty in exactly prescribing a given wave spectrum in a PiC experiment. This amplitude 372 $((B_{\rm w,rms}/B_0)^2 \approx 3 \times 10^{-8})$ still falls well below the nonlinear wave amplitude thresholds 373 as discussed in Section 1. Therefore, this factor does not preclude us from comparing our 374 results to those obtained by Tao et al. [2011]. As discussed above, we excite the boundary 375 with individual whistler modes each with electric field amplitudes that correspond to mag-376 netic field perturbations of 1pT, but for the case of a vacuum $(|\delta \mathbf{B}| \approx |\delta \mathbf{E}|/c)$. However, 377 when propagating through a plasma medium, one will expect magnetic field perturbations 378 within the domain $|\delta \mathbf{B}| \approx |\delta \mathbf{E}|/(c/\eta)$ (in our experiment 14.8 < η < 18.1 for waves 379 with frequencies $f_{\rm lc} < f < f_{\rm uc}$). If the coupling efficiency between the wave excitation 380 mechanism and the plasma was 100% efficient, then we should expect a spectrum of mag-381 netic field perturbations (i.e. at each frequency) with amplitudes a factor of η greater than 382 $|\delta \mathbf{E}|/c$, i.e $\approx \eta \times 1$ pT. However, the coupling is not perfectly efficient, as should be ex-383 pected, and so we observe magnetic field perturbations within the domain $\approx 2-3$ times the 384 1pT level used by Tao et al. [2011]. One obtains near-identical results as those in figure 3 385 for the power spectra of the B_z and E_z components, as should be expected for circularly 386 polarized waves. 387

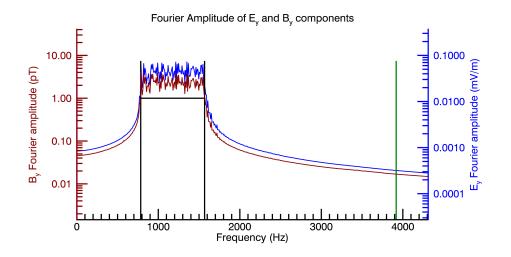


Figure 3. Fourier amplitude of the B_y (red) and E_y components (blue) of the waves within the PiC domain. Vertical black lines mark the lower and upper bounds of the driven wave spectrum ($f_{lc} = 0.2 f_{ce}$ and $f_{uc} = 0.4 f_{ce}$ respectively). Vertical green line marks the electron gyrofrequency f_{ce} . The horizontal black line marks a continuous version of the B_y spectrum employed by *Tao et al.* [2011].

Figure 4 shows the 'dispersion relation' of the B_y component of the waves present, obtained via Fourier transforms performed over the entire spatial and temporal domain during the wave-particle interaction. The over-plotted line marks the cold plasma dispersion relation as according to equation (1), and we see that the dominant power is strongly localized to the (f_{lc}, f_{uc}) region, and along the expected dispersion curve. Once again, we obtain near-identical plots of the dispersion relation for B_z, E_y and E_z .

394 3 Particle diffusion

The application of QLT to the Vlasov-Maxwell equation for collisionless plasmas leads to a diffusion equation to describe the plasma distribution function, F, of the form

$$\frac{\partial F}{\partial t} = \sum_{i,j} \frac{\partial}{\partial J_i} \left[D_{ij} \frac{\partial F}{\partial J_j} \right]$$
(3)

[Schulz and Lanzerotti, 1974], for D_{ij} a symmetric tensor of diffusion coefficients, and J_i 397 are the three action integrals associated with adiabatic charged particle motion [Northrop, 398 1963; Roederer and Zhang, 2013]. For use in the outer radiation belt, equation (3) is typ-399 ically rewritten in (E, α, L^*) space (e.g. see *Glauert et al.* [2014]). Here, the energy E =400 $p^2/(2m_{0e})$ (for $\mathbf{p} = \gamma m_{0e} \mathbf{v}$, with γ the relativistic gamma, and m_{0e} the electron rest mass); pitch angle $\alpha = \tan^{-1}(|p_{\perp}/p_{\parallel}|)$ (for p_{\perp} and p_{\parallel} the momenta perpendicular and parallel to 402 the background magnetic field); and $L^{\star} \propto 1/\Phi$, is a value inversely proportional to the 403 third adiabatic invariant [Roederer and Zhang, 2013; Roederer and Lejosne, 2018]. The 404 work in this paper does not consider radial diffusion (i.e. diffusion in L^*). It is the diffu-405 sion in pitch angle, characterized by $D_{\alpha\alpha} = D_{\alpha\alpha}(E, \alpha)$, that will be the focus. 406

Particles are considered to be in resonance with a given wave mode when the waveparticle resonance condition is satisfied [*Kennel and Engelmann*, 1966],

$$\omega - k_{\parallel} v_{\parallel} = n \omega_{\rm ce} / \gamma. \tag{4}$$

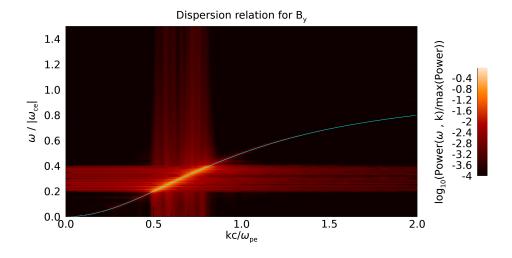


Figure 4. 'Dispersion relation' of the B_y component of the waves present in the numerical experiment, averaged over the entire spatial and temporal domain during the wave-particle interaction. The over-plotted cyan curve marks the cold plasma dispersion relation (see equation (1)).

In this equation, $\omega > 0$ is the wave frequency, $n = 0, \pm 1, \pm 2, ...; k_{\parallel} = \mathbf{k} \cdot \mathbf{B}_0/B_0$ and $v_{\parallel} = p_{\parallel}/(m_{0e}\gamma)$ are the wave vector and velocity components that are parallel to B_0 , and we remind that $\omega_{ce} < 0$. In the case of field-aligned whistler mode waves, only the n = -1resonance can occur for electrons (e.g. see *Summers* [2005]). Under these circumstances, wave-particle resonance occurs for a given wave frequency, ω , for pitch angles and energies defined by

$$\alpha = \cos^{-1}\left(\left|\frac{|\omega_{ce}|/\omega - (1+\varepsilon)}{(kc/\omega)\sqrt{\varepsilon^2 + 2\varepsilon}}\right|\right),\tag{5}$$

for $\varepsilon = E/(m_{0e}c^2)$, and kc/ω given by equation (1). This equation implies that for a given pitch angle, lower frequency waves resonate with higher energies [*Camporeale*, 2015; *Chen et al.*, 2018]. Furthermore, for a given wave frequency, the values of particle energy that can resonate are a monotonically increasing function of pitch angle.

419

3.1 Background theory on normal diffusion

An implicit assumption in the use of QLT is that the plasma undergoes 'normal diffusion' [*Bouchaud and Georges*, 1990] in phase-space: "*the diffusion model assumes the existence of an underlying uncorrelated, Gaussian stochastic process, i.e., a Brownian random walk*" [*del Castillo-Negrete et al.*, 2004]. In this normal diffusive framework, diffusion coefficients are defined by the following formula (for arbitrary variables X and Y),

$$D_{XY}(X,Y) = \frac{\langle \Delta X_l \rangle \langle \Delta Y_l \rangle}{2\Delta t},\tag{6}$$

in units of $[X][Y]s^{-1}$. Here, Δt is interpreted as the duration over which the diffusion coefficients are to be calculated, X_l and Y_l are distributions of the particle parameters, localized to given values of X and Y (for N particles l = 1, 2, ..., N within the given local population). The mean of the distribution X_l is denoted by $\langle X_l \rangle$, and

$$\langle \Delta X_l \rangle \equiv \langle X_l - \langle X_l \rangle \rangle, \tag{7}$$

such that $\langle \Delta X_l \rangle^2 \equiv \operatorname{var}(X_l)$, for $\operatorname{var}(X_l)$ the variance of the distribution X_l . Implicit within this normal diffusion construction, is that the variance of a given parameter scales linearly with time,

$$\Delta \operatorname{var}(X_l) = 2D_{XX} \Delta t,$$

(8)

for $\Delta \text{var}(X_l)$ the change in the variance of X_l over the time Δt (e.g. see *Bouchaud and Georges* [1990]; *Metzler and Klafter* [2000]). Conceptually, this means that for a given subset of a plasma population that is located in some region of phase space, then the distribution of that subset will spread in phase space according to equation (8).

436 **4** Diffusion in our numerical experiments

Particle diffusion due to wave-particle interactions is monitored by using the EPOCH 437 'tracer' particle feature. EPOCH allows the embedding of test-particle populations (trac-438 ers) into numerical experiment. Unlike all the other particle populations, tracer particles 439 do not contribute to the current, and so they effectively act as labels in phase-space: that 440 is to say that the behaviour of a given tracer is indicative of the behaviour of an interact-441 ing particle (one that does contribute moments) in the same given region of phase-space. 442 We release $\approx 10^8$ tracer particles within the domain at t = 0, that are initially distributed 443 according to a 100keV Maxwellian distribution that is uniform in space. Since they do 444 not contribute current, we can load tracers however we want in phase space. We choose 445 this specific 'temperature' merely to provide a relatively uniform distribution of particles across the section of energy space important for pitch-angle diffusion in the Radiation 447 Belts. 448

Once the driven wave profile crosses the experimental domain, we consider all of 449 the tracer particles to be under the influence of the whistler-mode waves. At $t = t_{cross}$, 450 we bin the tracer particles in two dimensions according to their values of energy and pitch 451 angle at that time. We emphasize that tracers then remain identified with that given bin 452 for the entirety of the experiment, i.e. we do not re-bin at each data-dump. The binning 453 process is performed as follows. We first order all of the $\approx 10^8$ tracers according to their energy at $t = t_{cross}$, and separate these tracers into 250 intervals, which are defined so as to 455 allow exactly identical numbers of tracers in each interval. Within each of these energy in-456 tervals, the tracers are then ordered according to their value of pitch angle, and subdivided 457 into 90 pitch angle sub-intervals, defined in order to allow the same number of tracers in 458 each. Each of these 250×90 bins in energy and pitch-angle space contains 4444 tracer par-459 ticles, and therefore we have uniformly good statistics within each bin with which to cal-460 culate the diffusive response. In the case of an isotropic Maxwellian distribution, it would 461 be expected that this procedure would yield bins of a uniform size in pitch angle space, 462 within each energy interval. Our bins are not exactly uniform in pitch angle space, but 463 they are almost uniform. The reason is as follows. The tracer particles are loaded into the 464 simulation at t = 0 as an isotropic Maxwellian. However, they are binned at a later time, 465 $t = t_{cross}$. Between t = 0 and $t = t_{cross}$, the tracers have been responding to the electromag-466 netic perturbations within the domain created by both the wave excitation mechanism and 467 any other inherent PiC electromagnetic fluctuations, and therefore the tracers are not be in 468 a perfectly isotropic state at $t = t_{cross}$. 469

4.1 Scattering in phase-space

470

Figure 5 shows an example of the diffusive response for particles within a bin roughly 471 centred on $\alpha = 75^{\circ}$ and E = 50 keV. This combination of energy and pitch angle im-472 plies that the particles are in resonance with the driven wave spectrum. From hereon in 473 we redefine $t = t_{cross}$ as $\tilde{t} = 0$, and the end of the simulation as $\tilde{t} = T$, to simplify the 474 discussion. Figures 5(a)-(d) plot electron E, α values at $\tilde{t} = 0, T/3, 2T/3$ and $\tilde{t} = T$ re-475 spectively, and figures 5(e)-(h) plot pitch angle distributions of the entire sub-population 476 (all energies). It is evident that pitch-angle diffusion dominates over energy diffusion in 477 this bin, for reasoning as follows. The maximum magnitude of the pitch angle scattering 478 in this bin reaches values of $(\max(\Delta \alpha))^2/(2T) \approx (\pm 3)^2/(2T) = 9/(2T)$. Whereas the en-479

ergy scattering in this bin reaches maximum magnitudes of $(1/E^2)(\max(\Delta E))^2/(2T) \approx$ 480 $(1/50 \text{keV})^2 (\pm 1 \text{keV})^2 / (2T) = 0.0004 / (2T)$. We have checked that the dominance of pitch-481 angle scattering is observed in most bins. This is an expected result, since the ratio $f_{\rm pe}/f_{\rm ce}$ 482 is known to control the relative significance of energy versus pitch angle diffusion [Sum-483 mers, 2005]. It is also interesting to note that the particles are scattered in preferred di-484 rections. This scattering is such that positive changes in E correlate with positive changes 485 in α , and negative changes in E correlate with negative changes in α . We have observed 486 that this behaviour is ubiquitous for the particles that are in resonance with the dominant 487 whistler-mode waves, and therefore the particles which undergo 'significant diffusion' (see 488 section 4.3 for a discussion on this topic, and our definition of 'significant diffusion'). The 489 observed scattering in a preferred direction is an expected result due to the following argu-490 ment. During a resonant interaction with a given parallel-propagating whistler-mode wave 491 $(\omega_k < |\omega_{ce}|)$, then (in the rest frame of the wave) an electron will experience changes in 492 the total kinetic energy, ΔE , and the perpendicular kinetic energy, ΔE_{\perp} , that are related 493 according to 494

$$\Delta E_{\perp} / \Delta E = |\omega_{\rm ce}| / \omega_k > 1, \tag{9}$$

(e.g. see equation (36) in *Brice* [1964]). Equation (9) implies that (in the rest frame of the wave) for a given positive change in the electron energy ($\Delta E > 0$), such that

$$\Delta E = \Delta E_{\perp} + \Delta E_{\parallel}$$

then the perpendicular energy must increase by a greater amount, i.e. $\Delta E_{\perp} > \Delta E$. Therefore the parallel energy must decrease ($\Delta E_{\parallel} < 0$). This therefore implies that the pitch angle must increase. One can use an exactly analogous argument using equation (9) to conclude that a decrease in the energy of an electron ($\Delta E < 0$) is consistent with a decrease of the electron pitch angle. These, and other, helpful observations are summarized in Table 1. of *Brice* [1964], and can also be seen clearly in Figure 1. from *Kennel and Petschek* [1966].

Furthermore, we see from Figure 5 that the particle population spreads from an initial 'top-hat' sample, into a Gaussian-type distribution. This property seems broadly consistent with the diffusive paradigm, in which initially localized distributions spread into Gaussian distributions with ever greater widths (variances).

4.2 The diffusive hypothesis

The direct evaluation of the nature of diffusion in response to a given wave spectrum, relies on both the plasma and wave characteristics being quasi-static for the time considered, Δt [*Schulz and Lanzerotti*, 1974]. Further to this requirement, we propose some additional constraints that are described by the following hierarchy of timescales,

$$\tau_{\text{wave}} \ll \Delta t \le \tau_{B(\omega,k)}, \ \tau_{n,B_0}, \ \tau_{\text{local}}, \tag{10}$$

that should be satisfied in order for one to directly measure properties of the diffusion for a given (E, α) bin. Equation (10) states that one can meaningfully evaluate diffusion due to interactions with a given wave frequency over timescales: (i) significantly larger than $\tau_{\text{wave}} = 1/f_{\text{wave}}$;(ii) smaller than those for which one observes variations in the wave spectrum ($\tau_{B(\omega,k)}$); (iii) and smaller than those for which one observes variations in the the background magnetic field and number density (τ_{n,B_0}). These conditions hold for our experiment.

Furthermore, in order to be able to consider the rate of diffusion as a function of Eand α over some timescale Δt , each given sub-population (or bin) of particles must remain localized to the same given region of (E, α) space for the duration of Δt . To be clear, consider one particular bin composed of l = 1, 2, ..., N particles, with initial values binned

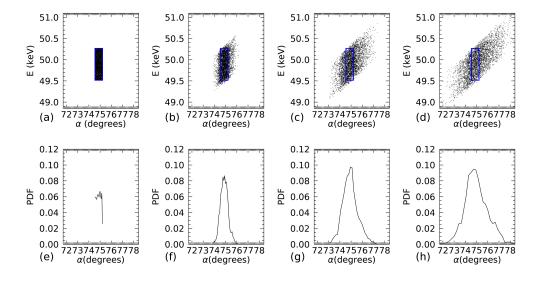


Figure 5. The diffusive response for 4444 electrons, within a bin roughly centred on 75° and 50keV. (a)-(d) plot electron *E*, α values at $\tilde{t} = 0$, *T*/3, 2*T*/3 and $\tilde{t} = T$ respectively. (e)-(h) plot pitch angle distributions of the given particles at those times.

according to $[(E_{\text{bin, min}} < E_l(t = 0) < E_{\text{bin, max}}), (\alpha_{\text{bin, min}} < \alpha_l(t = 0) < \alpha_{\text{bin, max}})]$. Then, in order to be able to measure diffusion for that given bin, we require

$$E_{\text{bin, min}} < \langle E_l \rangle(\tilde{t}) < E_{\text{bin, max}},$$

$$\alpha_{\text{bin, min}} < \langle \alpha_l \rangle(\tilde{t}) < \alpha_{\text{bin, max}}.$$
(11)

We define the timescale over which $\langle E_l \rangle(t)$ and $\langle \alpha_l \rangle(\tilde{t})$ satisfy the above constraints in a given bin as τ_{local} . Therefore, if satisfied, then the electrons in the given bin undergo negligible advection in (E, α) space over the timescale τ_{local} .

532

Figure (6) plots a normalized measure of local advection in phase-space,

$$d\alpha(E,\alpha) := \frac{\Delta\langle \alpha_l \rangle}{|\operatorname{bin}(\alpha_l)|}.$$
(12)

Here, $\Delta \langle \alpha_l \rangle = \langle \alpha_l \rangle (\tilde{t} = T) - \langle \alpha_l \rangle (\tilde{t} = 0)$, and $|bin(\alpha)| = \alpha_{bin, max} - \alpha_{bin, min}$. The 533 over-plotted white curves mark the values of energy and pitch angle that are (according 534 to equations (4) and (5)) in "n = -1 resonance" with waves of frequency f_{lc} ('dash'), f_{uc} 535 ('dash-dot'), and $(f_{lc} + f_{uc})/2$ ('solid'). We can see that the largest values of $d\alpha$ are lo-536 calized to regions within the boundaries of the resonance curves, and have maximum size 537 less than 0.5 (max($|d\alpha|$) \approx 0.36). Therefore, for this choice of binning, all electron sub-538 populations remain localized to their given pitch-angle bins for the duration of the interaction that we consider, $0 < \tilde{t} < T$. Therefore an evaluation of diffusive properties is valid, 540 i.e. timescales are in agreement with equation (10) and the diffusive hypothesis holds over 541 the given timescale $\Delta t = 460t_{ce}$. We have also constructed a similar plot for dE, which 542 shows qualitatively similar results (max(|dE|) ≈ 0.25), and so sub-populations also remain 543 localized to their given energy bins. 544

548 **4.3** Nature of the diffusion

As described at the beginning of Section 3, the calculation of a diffusion coefficient (e.g. $D_{\alpha\alpha}$) within the normal diffusive paradigm assumes that the variances of electron

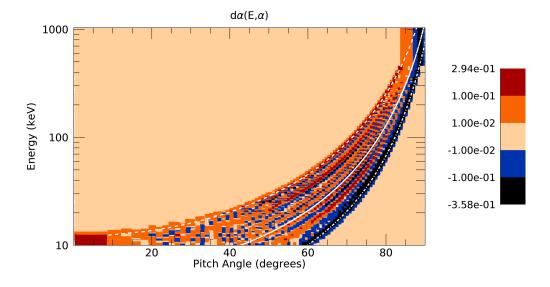


Figure 6. $d\alpha(E, \alpha)$, for each (E, α) bin in the experiment (see equation (12)). The over-plotted white curves mark the values of energy and pitch angle that are (according to equations (4) and (5)) in "n = -1 resonance" with waves of frequency f_{lc} ('dash'), f_{uc} ('dash-dot'), and $0.5(f_{lc} + f_{uc})$ ('solid').

pitch-angle distributions within a given bin grow linearly with time. In this case, the diffusion coefficient is given by equation (8), and defines the slope of the line according to var(α_l) = $2D_{\alpha\alpha}\Delta t$. Prior to calculating diffusion coefficients, it is therefore important to check whether the data supports this implicit assumption of 'variances that grow linearly in time'.

Figures 7(a)-(c) plot the evolution of $var(\alpha_l)$ for three different example bins. These 559 bins are given by $(E, \alpha) = (20 \text{keV}, 45^\circ)(300 \text{keV}, 82^\circ)$, and $(50 \text{keV}, 75^\circ)$. The asterisks 560 mark the directly extracted particle data, and the solid black lines mark curve fits. The 561 curve-fitting method is described in Appendix B. For the purposes of presentation, the par-562 ticle variance curves are translated so that $var(\alpha_l; \tilde{t} = 0) = 0$. An instantaneous measure 563 of the rate of diffusion could be considered to be $d(var(\alpha_l))/d\tilde{t}$. Figure 7(b) shows an example for which this rate of diffusion appears to be roughly constant in time. However, 565 figures 7(a) and 7(c) show examples for which the rate appears, respectively, to be slowing 566 down and speeding up as time passes. This time-dependent rate of diffusion is an interest-567 ing feature, and does not (at first glance) appear consistent with the assumptions of normal diffusion theory. Diffusive theories that move beyond the assumption of normal diffusion 569 (sometimes called 'anomalous diffusion') have many applications, and not only in space 570 physics (e.g. see Bouchaud and Georges [1990]; Metzler and Klafter [2000]; Zaslavsky 571 [2002]; Perrone et al. [2013]; Zimbardo et al. [2015]). Anomalous diffusion theory essen-572 tially allows for the variance of a given parameter X to evolve according to a power-law 573

$$\operatorname{var}(X_l) \propto t^a,$$
 (13)

for $0 < a < \infty$, and for which a < 1 denotes 'sub-diffusion', $a \approx 1$ denotes 'normal diffusion', and a > 1 denotes 'super-diffusion'. Using this interpretation, figures 7(a)-(c) present values a = 0.52, a = 0.92 and a = 2.21 respectively (suggesting sub-, normal- and super-diffusion respectively). It is interesting to see that the diffusion observed does not always follow normal diffusive behaviour over the time-scales $0 < \tilde{t} < T$. Each sub-figure also includes a blue solid line, obtained via imposing a linear fit to the raw data over the second half of the wave-particle interaction, $T/2 < \tilde{t} < T$. These straight lines are a good fit in each case. This suggests that normal diffusion is observed in all three cases, but only after an initial transient phase during which anomalous diffusion occurred.

Figure 8 plots the evolution of $var(\alpha)$ for a bin roughly centred on $(E, \alpha) = (9.2 \text{keV}, 40^\circ)$. 583 This sub-population of particles is resonant with waves of frequency $f = 0.3 f_{ce}$, and rep-584 resents a direct comparison with the main example plotted by Tao et al. [2011] (figure 2 585 in that paper). The black and blue solid lines represent the same curve fits as applied to 586 figure 7. The solid green line represents the theoretical evolution of $var(\alpha)$, as inferred by 587 using the value of $D_{\alpha\alpha}$ as predicted from the PADIE code [Glauert and Horne, 2005] us-588 ing input plasma and wave parameters as detailed in this paper. As a reminder, note that $var(\alpha) = 2\Delta t D_{\alpha\alpha}$ under the assumption of normal diffusion. The diffusion index for this 590 bin is given by a = 1.15 and therefore classified as normal diffusion. We see a very good 591 agreement between the theoretical diffusion coefficient and our directly extracted data on 592 the diffusive response for this particular energy and pitch-angle bin. We will follow up on 593 direct comparisons between $D_{\alpha\alpha}$ as predicted from the PADIE code and diffusive response 594 in our PiC experiments in a separate paper that will include all energy and pitch-angle 595 bins. 596

Figure 9 presents contour plots of the diffusion index, a, for each (E, α) bin, as defined in equation (13). We remind that we calculate the value a for each and every bin over all phase space ($0 < \alpha < 90$, 9keV < E < 1MeV). The rate of diffusion that is observed is a function of phase-space, and we observe very weak diffusion in some bins. We do not present the value of a when diffusion is very weak, and instead mask those cases with black. For this purpose, a measure of the strength of the diffusion is calculated as follows. We calculate the total change in the variance of the pitch-angle distributions within each bin,

$$D_{\alpha\alpha,\text{proxy}}(E,\alpha) = \frac{\operatorname{var}(\alpha_l; \tilde{t} = T) - \operatorname{var}(\alpha_l; \tilde{t} = 0)}{2T}.$$
(14)

Significant diffusion is deemed to have occurred within a given bin, if the value of this diffusion proxy satisfies

$$D_{\alpha\alpha,\text{proxy}}(E,\alpha) > 10^{-2} \max_{E,\alpha} \left\{ D_{\alpha\alpha,\text{proxy}}(E,\alpha) \right\}.$$
 (15)

If significant diffusion does occur, then we describe its nature as 'sub-diffusion' if < a <610 0.67 by using yellow, as normal diffusion if 0.67 < a < 1.5 by using pink, or as 'super-611 diffusion' if a > 1.5 by using dark-red. These bounds of $a < a_{sub} = 2/3$ and $a > a_{super} =$ 612 $1/a_{sub}$ were chosen in order to classify sub- and super-diffusion relatively strictly. Any re-613 gions for which the curve-fitting routine failed, are represented by missing data (white). 614 As was done for figure 6, the over-plotted cyan curves mark the values of energy and 615 pitch angle that are in "n = -1 resonance" with the driven waves. Furthermore, the locations of the bins represented in figure 7(a)-(c) are marked by cyan symbols: "<", " \star " and 617 ">" respectively. Figure 9(a) shows the value of a that is calculated over the entire wave-618 particle interaction (0 < t < T). One clear observation is that the regions of significant 619 diffusion, as defined by equation (15), are almost exclusively localized within the "n = -1resonance" regions of phase space. Figure 9(a) also shows two well-defined region of sub-621 and super-diffusive behaviour. The sub-diffusive region is found at 'lower-frequency' res-622 onances, and predominantly lower energies (< 100keV); whereas the super-diffusive be-623 havior is observed for 'higher-frequency' resonances, and across the entire energy range. 624 Out of all bins in which significant diffusion was observed, 7.2% show sub-diffusion, 45%625 show normal-diffusion, and 47.8% show super-diffusion. 626

Figure 9(b) shows the same quantity as figure 9(a), but calculated over the secondhalf of the interaction $(T/2 < \tilde{t} < T)$. This plot is motivated by the hypothesis made after analysis of figures 7(a)-(c), that an initial transient period of varying diffusion rates gives way to normal diffusion in the latter half of the experiment. We indeed see from figure 9(b) that a smaller proportion of the plot (i.e. fewer bins) displays the sub- and superdiffusive behaviour. This observation is consistent with the observations made of the data ⁶³³ in figures 7(a)-(c): during $0 < \tilde{t} < T/2$ we observe an initial transient phase during which ⁶³⁴ different kinds of diffusive responses are possible; later on (during $T/2 < \tilde{t} < T$) we ob-⁶³⁵ serve a shift towards a normal-diffusive response. Out of all bins in which meaningful dif-⁶³⁶ fusion was observed, 2.9% show sub-diffusion, 86.7% show normal-diffusion, and 10.4% ⁶³⁷ show super-diffusion during the second half of the numerical experiment.

646 **5 Discussion**

We use the EPOCH particle-in-cell code [Arber et al., 2015] to track electron pitch-647 angle diffusion due to interactions with whistler-mode waves. There are two main novel 648 features to our approach: (i) we consider diffusion using a PiC code as a boundary value 649 problem, i.e. we excite specific wave modes at the boundary, as opposed to considering an 650 initial-value problem in which one typically considers waves that grow from an initially 651 unstable distribution (e.g. see Katoh and Omura [2006]; Omura et al.; Hikishima et al. 652 [2009]; Omura et al. [2009]; Omidi et al. [2010, 2011]; Katoh and Omura [2013]; Cam-653 poreale [2015]; Camporeale and Zimbardo [2015]; Silva et al. [2017]; Ratcliffe and Watt 654 [2017]; Katoh et al. [2018]); (ii) by considering the response of a distribution of electrons, 655 we track the diffusion in energy and pitch angle space across the entire phase-space do-656 main, in contrast to some previous similar studies of diffusion (e.g. see *Tao et al.* [2011, 657 2012a]; Camporeale and Zimbardo [2015]) that considered resonant particles only. These novel features allow us to, respectively: (i) consider a 'quasi-static' system, in which the 659 background plasma and whistler-mode wave spectra are roughly time-independent; (ii) 660 derive characteristics of the diffusive response for all electrons, including those that are 661 non-resonant with the waves and typically not expected to strongly interact.

In this first study, we model the background plasma as a 0.1eV isotropic cold popu-663 lation. We use this approach to benchmark our novel method with expected results, before studying more realistic 'radiation belt' background plasmas in the future, with 'warm' and 665 'hot' anisotropic electron populations (see e.g. Denton et al. [2010]). We also make the 666 assumption of spatially 1D dynamics, thereby permitting only parallel and anti-parallel 667 wave propagation, as well as a homogeneous background magnetic field. This consider-668 able simplification is done in order to benchmark with previous work [Tao et al., 2011], 669 and with a mind to a systematic future program of work with more realistic magnetic field 670 geometries, wave-normal-angle spectra, and/or more 'exotic' wave modes and amplitudes. 671 In order to properly understand each effect, it is necessary to first understand the experi-672 mental response in the most simple of circumstances, and then implement additions in iso-673 lation. We have compared our results for pitch angle diffusion with the example presented 674 by Tao et al. [2011], using results from the PADIE code, and we see very good agreement. A more comprehensive comparison of the diffusive response with the predictions of QLT 676 is beyond the scope of this paper, but will be addressed explicitly in future papers in this 677 series. 678

Extremely low levels of background noise have been enabled by using the δF mode 679 in EPOCH. This, in addition to the linear envelope applied to the wave driver, allows for 680 a highly effective wave-driving mechanism for whistler-mode waves, with an excellent signal-noise-ratio. We have verified that the wave power is well localized to follow the 682 cold plasma dispersion relation. A large number of tracer particles were embedded within 683 the PiC domain ($\approx 10^8$ electrons) by using the EPOCH tracer functionality. This provides 601 good statistics with which we characterize the electron diffusion over the entire energy and 685 pitch angle domain. The dominant diffusion is clearly seen to correspond to those parti-686 cles that are in 'n = -1' resonance with the driven wave mode, as expected by QLT. Dif-687 fusive effects outside the resonant regions of phase-space are at most 1% as significant as 688 the dominant resonant effects. Therefore, for this experiment, non-resonant interactions are 689 of little importance (unlike in e.g. Camporeale [2015]). This feature is an explicit require-690 ment of QLT, and seems sensible given the simplified nature of the experimental setup. 691

Future investigations will seek to determine those circumstances under which nonlinear effects become more important.

One interesting feature of the diffusion is observed for early times; namely, a time-694 dependent rate of diffusion. The variances of pitch-angle distributions of given electron 695 sub-populations do not always grow linearly with time during the first half of the experiment (see figures 7 and 9). We discuss this result in the context of 'anomalous' diffusion 697 theories (e.g. see Bouchaud and Georges [1990]; Metzler and Klafter [2000]; Zaslavsky [2002]; del Castillo-Negrete et al. [2004]; Perrone et al. [2013]; Zimbardo et al. [2015]), 699 that are known to play a role in various space and astrophysical plasma contexts. How-700 ever, at later times, normal diffusion (Brownian motion) is seen to dominate, during which 701 time the variances grow with a linear rate. This latter result is consistent with the implicit 702 assumptions of QLT, and suggests that in order to construct meaningful diffusion coeffi-703 cients from such PiC experiments, one may have to consider how to appropriately treat 704 this initial transient phase (see examples of possible methods to treat time-dependent diffu-705 sion rates in e.g. *Degeling et al.* [2007]). 706

707 6 Summary

In this first paper of a series, we analyze the nature of the electron pitch-angle dif-708 fusion due to interactions with broadband and incoherent whistler-mode waves. The most 709 significant technical development is a proof-of-concept for the novel method used. Namely, 710 an analysis of the nature of electron diffusion over all phase-space due to specified whistler-711 wave modes, using a particle-in-cell method to construct a boundary-value problem. This 712 analysis is enabled by direct extraction of particle data from numerical experiments per-713 formed using the EPOCH code. The numerical experiment was intended to both resemble and build upon the test-particle experiments performed by *Tao et al.* [2011]. As such, we 715 drove an incoherent spectrum of whistler-mode waves into a simple cold plasma with uni-716 form background magnetic field, and tracked the diffusive response of $\approx 10^8$ electrons for 717 460t_{ce}, as a function of energy and pitch angle. We make the following observations of 718 our experiments: 719

- 7201. The strength of the diffusive response is found to be a function of energy and pitch
angle, as is expected using quasilinear diffusion theory. The diffusion is strongest
in regions of energy-pitch angle space that are in the n = -1 resonance with the
dominant wave signal. This is not a new result, but a required one, since the only
wave-particle resonance that is possible in our experiment is the n = -1 case. How-
ever, it is an important benchmarking criteria that our novel method must satisfy,
and therefore it is important to check and present.
- Non-resonant interactions are observed to be of little consequence in this case. This
 feature is directly observed in our numerical experiments, and is not *a priori* assumed. It will be interesting to check how this feature changes in future experiments.
- 7313. When considered over the entire duration of the wave particle interaction for partic-
ular regions of energy-pitch angle space, the nature of the diffusive response is ob-
served in some regions of phase-space to be: (a) 'normal', i.e. it is Einsteinian/Brownian
(for which the variances of energy or pitch angle grow linearly with time, as is im-
plicit in QLT); (b) or 'anomalous', i.e. it is either super- or sub-diffusive (for which
the variances of energy or pitch angle grow at either a faster or slower relative rate,
respectively)
- 4. When considered over the second half of the wave-particle interaction, we observe that a larger proportion of phase-space exhibits a normal diffusive response due to the wave-particle interaction

741 742 743 5. A preliminary analysis of the strength of pitch-angle diffusion for a given region of energy and pitch angle space demonstrates consistency with the results presented by *Tao et al.* [2011], and the results of the PADIE code.

The results presented in this paper effectively benchmark our techniques against 744 other treatments that consider the response of test-particles to whistler-mode waves (e.g. 745 see *Tao et al.* [2011]). This work motivates the following future investigations on: (i) the 746 strength and nature of diffusion as a function of driving wave amplitude; (ii) the differ-747 ence in the plasma response when more realistic radiation belt plasmas are modelled, i.e. 748 those with the fractional warm components that can be found in Earth's inner magneto-749 sphere. It will also be interesting to consider methods that allow for a analysis of a fully 750 self-consistent electron response to whistler-mode waves, i.e. to move beyond the mixed 751 'PiC – test-particle approach' that we employed in this paper, and therefore beyond any of 752 its inherent limitations. 753

Beyond that, there are many questions remaining that motivate other future studies. 754 Namely, how do the results presented in this paper change when modelling other mani-755 festations of whistler-mode waves (e.g. monochromatic waves), other wave spectra (e.g. 756 with a much wider wave-normal angle spectrum). It will also be important to study the 757 diffusive response in spatially two-dimensional plasmas, with both homogeneous and inho-758 mogeneous background magnetic fields. Oblique waves can only propagate in a numerical experiment that has more than one spatial dimension, and are known to be relevant for 760 some properties of whistler-mode wave dynamics in the radiation belts (e.g. see Artemyev 761 et al. [2016a]; Ratcliffe and Watt [2017]). All of these effects should be expected to pro-762 duce qualitatively different diffusive responses. 763

764 A: The EPOCH particle-in-cell code

We use version 4.16 of the Extendable PiC Open Collaboration (EPOCH) code in 765 one spatial dimension ('EPOCH1D'). EPOCH is an explicit [Birdsall and Langdon, 2004], 766 relativistic and charge-conserving PiC code [Arber et al., 2015], using Villasenor and 767 Buneman current deposition [Villasenor and Buneman, 1992]. EPOCH solves Maxwell's 768 equations combined with the equations of motion for charged particles in an EM field to 769 provide a direct simulation of collisionless plasma. Since EPOCH uses an explicit scheme, 770 numerical stability requirements dictate that timesteps, Δt , are limited by the usual CFL 771 condition, and the resolution of electron plasma waves, for a given grid discretization Δx . EPOCH1D therefore sets the time scale as the most restrictive of constraints set by: the 773 CFL condition ($\Delta t_{CFL} = \Delta x/c$); the inverse plasma frequency, (at the beginning of the 774 simulation); and the inverse 'laser' frequency (the term 'laser' refers to an electromagnetic 775 wave driver), according to 776

$$\Delta t < \min(\Delta t_{CFL}, 1/(2f_{BG}), 1/(2f_{laser})),$$
 (A.1)

for $f_{BG} = |\omega_{BG}/(2\pi)|$ the ordinary frequency according to the Bohm-Gross dispersion relation [*Bohm and Gross*, 1949], and f_{laser} the minimum laser frequency. All quantities in EPOCH are given in normal SI units.

⁷⁸⁰ EPOCH allows users to run in ' δF mode'. In general terms, if we consider a plasma ⁷⁸¹ population as being described by a distribution function of the form $F = F_0(\mathbf{x}, \mathbf{v}) + \delta F(\mathbf{x}, \mathbf{v}, t)$ ⁷⁸² (with F_0 either an isotropic or anisotropic Maxwellian distribution function), then the ⁷⁸³ δF method (e.g. see *Sydora* [1999]) can achieve a reduction in PiC noise of the order of ⁷⁸⁴ $\sim |\delta F|/F$, for all other settings left unchanged. Hence, this method is particularly useful if ⁷⁸⁵ F is close to an (an-)isotropic Maxwellian distribution function.

⁷⁸⁶ Instructions on how to download and run EPOCH are given in supplementary infor-⁷⁸⁷ mation (S1).

B: Curve-fitting procedure

Here we describe the curve-fitting procedure, used to determine the diffusion index *a*, as shown in figures 7, 8 and 9. In each (E, α) bin, a time-series of the quantity

$$V_{\alpha}(\tilde{t}) = \frac{\operatorname{var}(\alpha_l; \tilde{t}) - \operatorname{var}(\alpha_l; \tilde{t} = 0)}{\operatorname{var}(\alpha_l; \tilde{t} = 0)},$$
(B.1)

⁷⁹¹ is calculated. We track V_{α} instead of just the variance, so that all time-series are ordinated ⁷⁹² according to similar scales, and are initialized at zero. This also helps with the curve-⁷⁹³ fitting procedure which is performed as follows:

(i) First, we test to see whether or not any 'significant diffusion' occurs in each bin, using the rule defined by equation (15). (ii) If significant diffusion occurred then curvefitting of the time-series, V_{α} , is implemented, to the test function,

$$y = c_0 + c_1 x^{c_2}$$

For a given initial estimate of the vector $\mathbf{c} = [c_0, c_1, c_2]$, the standard curve-fitting routine uses a gradient-expansion least-squares method, and returns a successful result when the relative decrease in chi-squared is less than 10^{-3} in a given iteration. The routine returns a fail if convergence is not reached after a large number of iterations, or if the chisquared value increases without bounds. Note that we classify 'successful' outputs of the curve-fitting algorithm as 'failures' if $c_2 > 10$, in order to neglect spuriously high values. Finally, curve-fitting could only be considered a success if $|y(x = 0)/y(x = x_{max})| < 0.5$.

(iii) For each bin, we employ this curve fitting routine for 100 different initial guesses of **c**, and record the output values of all 'successful' attempts. We then select the output vector that minimizes the mean deviation between the curve fit and the data. In theory, normal diffusion would give $c_2 \approx 1$, with the coefficient c_1 directly proportional to $D_{\alpha\alpha}$, and $c_0 = 0$.

Acknowledgments

The supporting information provides: (S1) basic instructions on how to run the same experiment that is presented in the main article; (S2) the contents of the input text file, used for the numerical experiment that is presented in the main article. This information will enable readers to locally generate the same experimental data as was considered in the main article.

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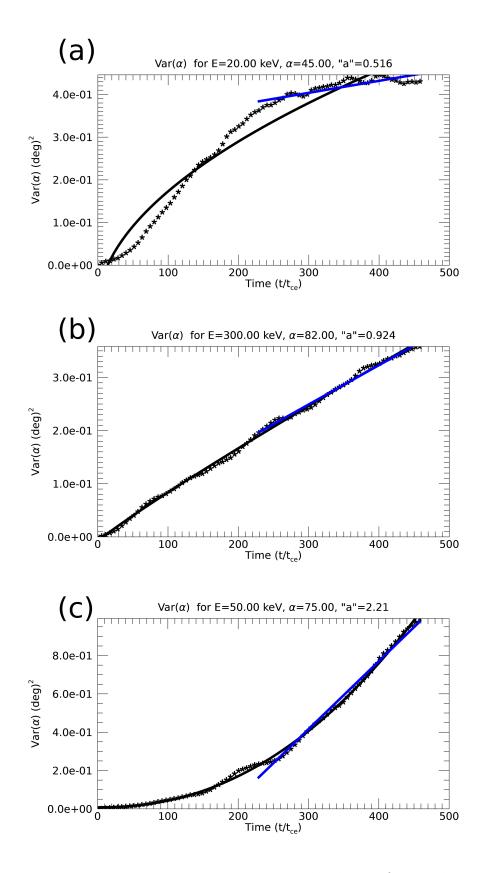


Figure 7. $var(\alpha_l)$ for three bins roughly centred on: (a): $(E, \alpha) = (20 \text{keV}, 45^\circ)$, (b): $(E, \alpha) = (300 \text{keV}, 82^\circ)$, and (c): $(50 \text{keV}, 75^\circ)$ respectively. Asterisks mark the particle data, and solid black lines mark curve fits. The solid blue line is a linear fit over $T/2 < \tilde{t} < T$.

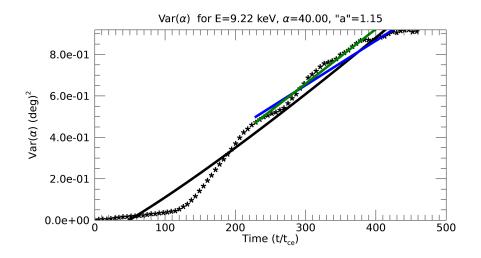


Figure 8. $var(\alpha_l)$ for a bin roughly centred on $(E, \alpha) = (9.2\text{keV}, 40^\circ)$. Asterisks mark the particle data, solid black lines is a curve fits, and the solid blue line is a linear fit over $T/2 < \tilde{t} < T$. The solid green line shows evolution of $var(\alpha)$ consistent with the PADIE diffusion coefficient, $D_{\alpha\alpha}$, over $T/2 < \tilde{t} < T$.

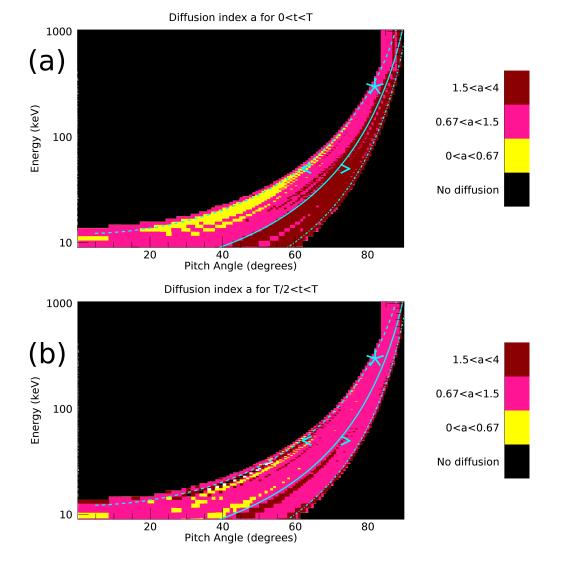
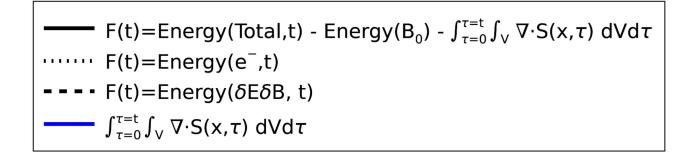


Figure 9. The diffusion index, a, for each (E, α) bin in the experiment. Plot(a) shows this index over the 638 entire time of wave-particle interaction $(0 < \tilde{t} < T)$, whereas plot (b) shows the index for the second half 639 of the interaction only $(T/2 < \tilde{t} < T)$. Black indicates 'no diffusion'. Yellow indicates 'sub-diffusion' 640 (0 < a < 0.67), pink indicates normal diffusion (0.67 < a < 1.5), and dark red regions indicate super-641 diffusion (a > 1.5). The over-plotted cyan curves mark the values of energy and pitch angle that are (accord-642 ing to equations (4) and (5)) in "n = -1 resonance" with waves of frequency f_{lc} ('dash'), f_{uc} ('dash-dot'), 643 and $0.5(f_{lc} + f_{uc})$ ('solid'). The bins represented in figure 7(a)-(c) are marked by cyan symbols: "<", " \star " and 644 ">". 645

Figure 1.



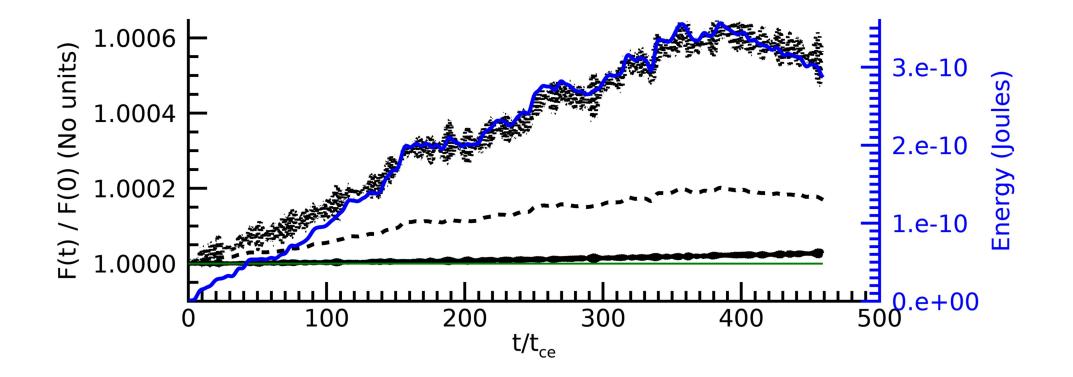


Figure 2.

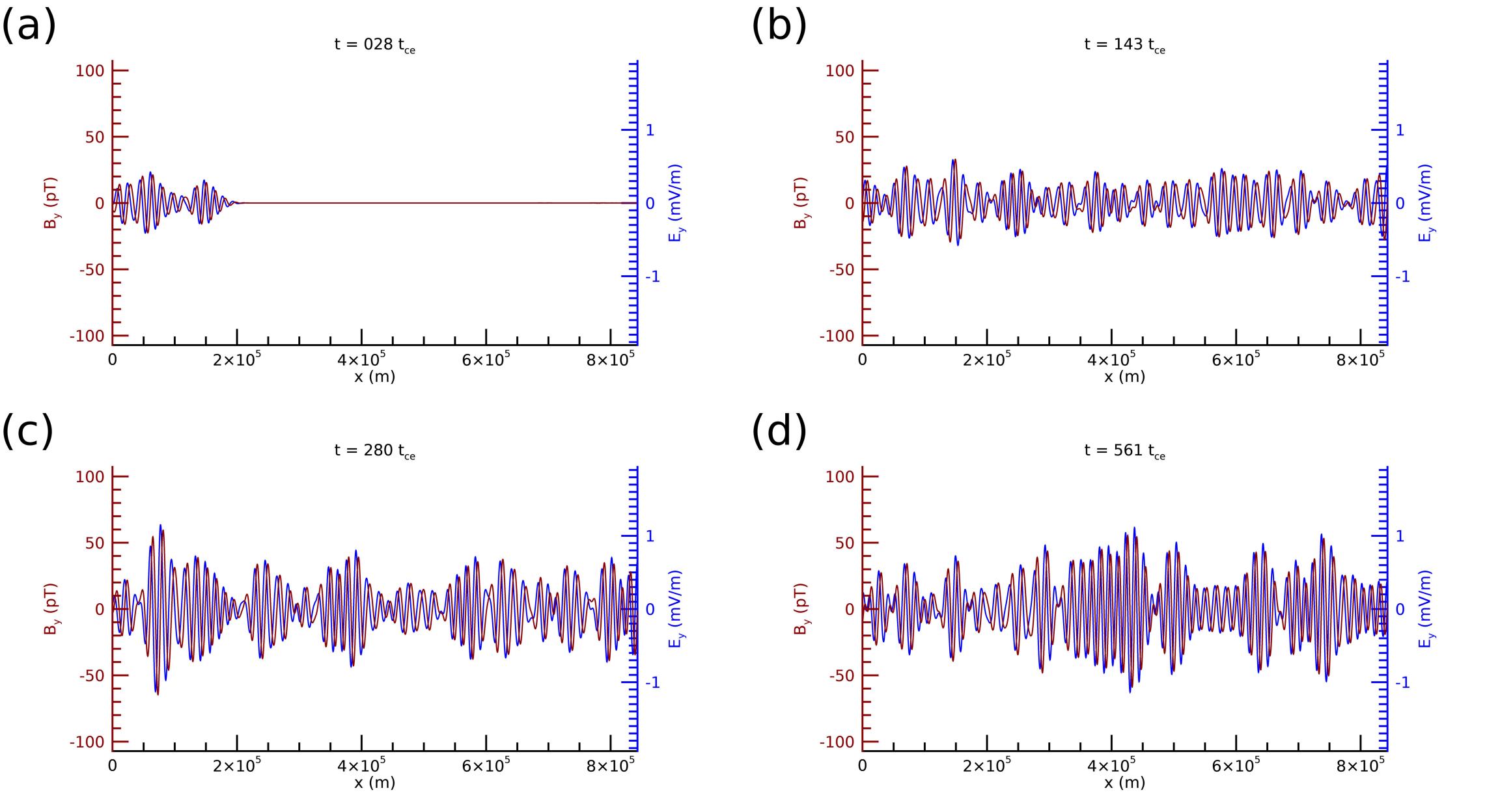


Figure 3.

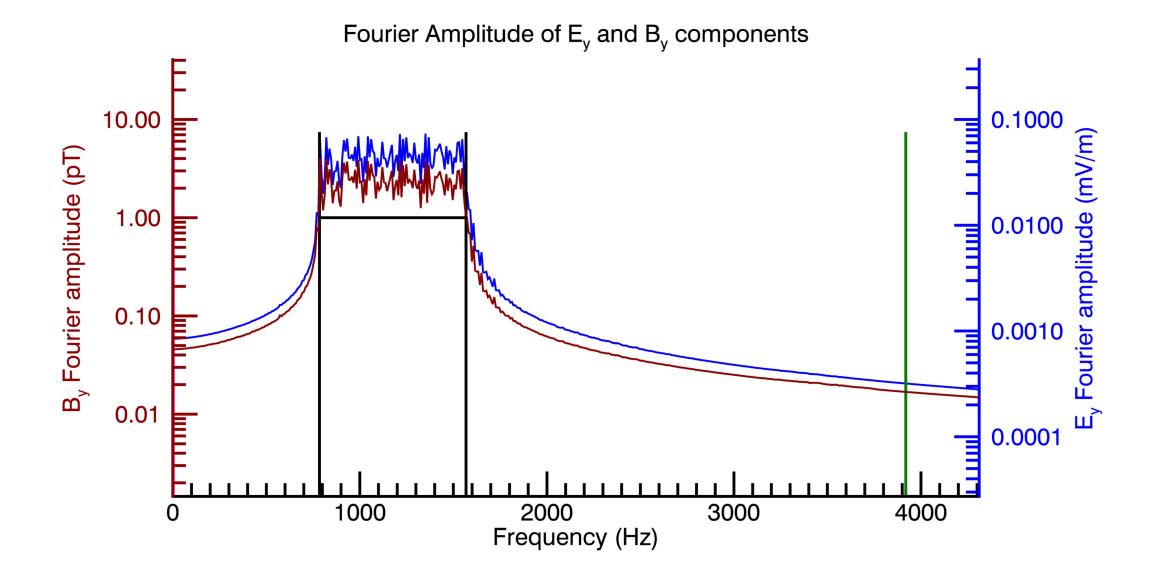
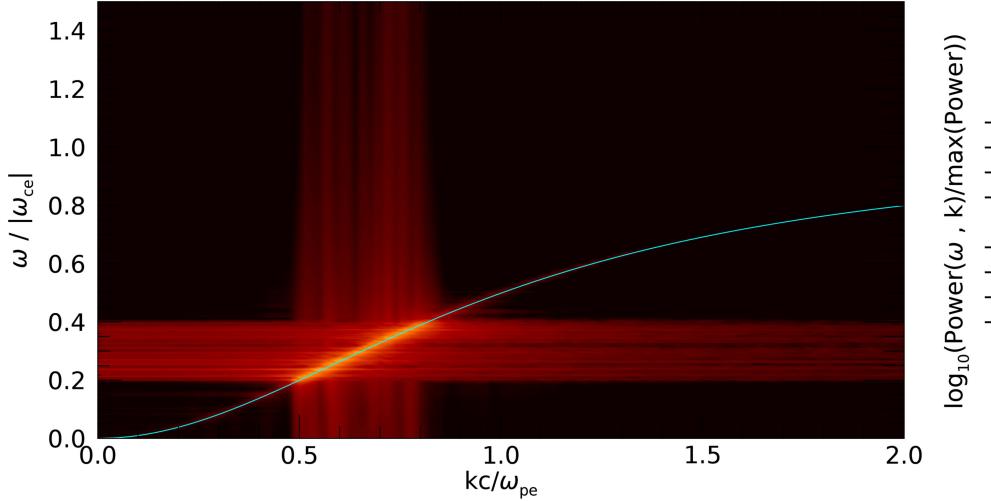


Figure 4.

Dispersion relation for B_v



-0.4 -0.8 -1.2 -1.6 -2 -2.4 -2.8 -3.2 -3.6 -4

Figure 5.

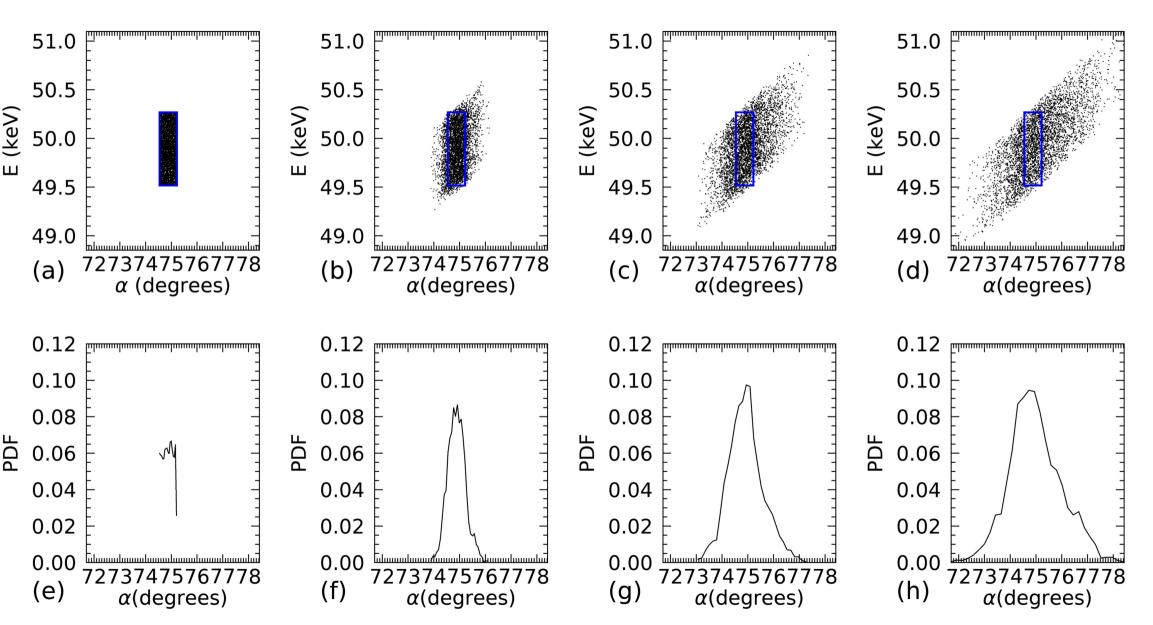


Figure 6.

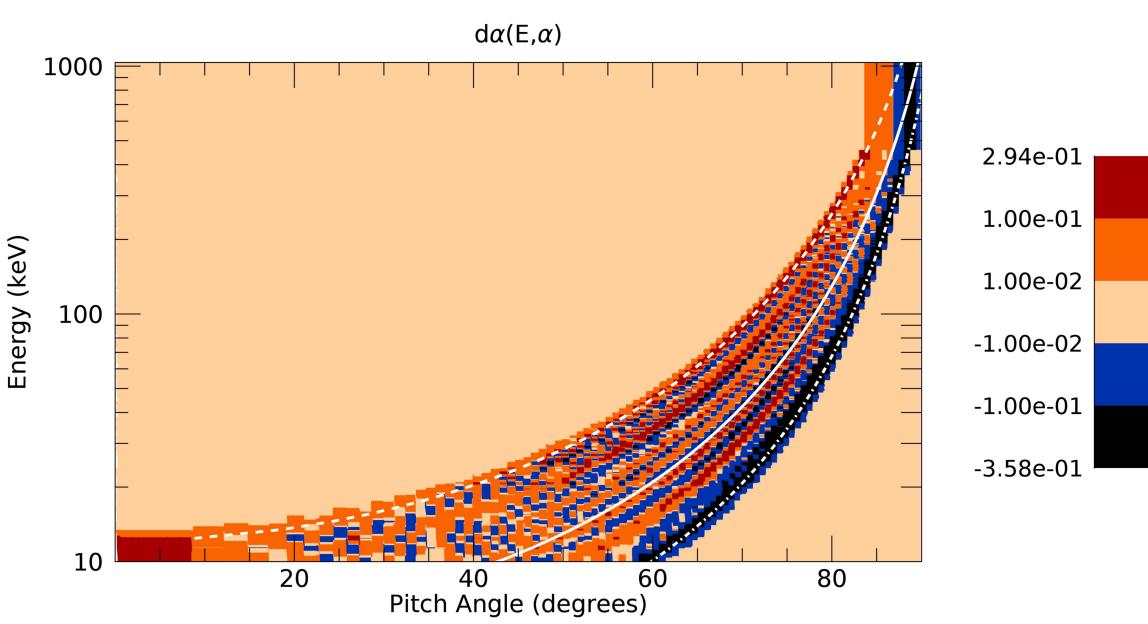
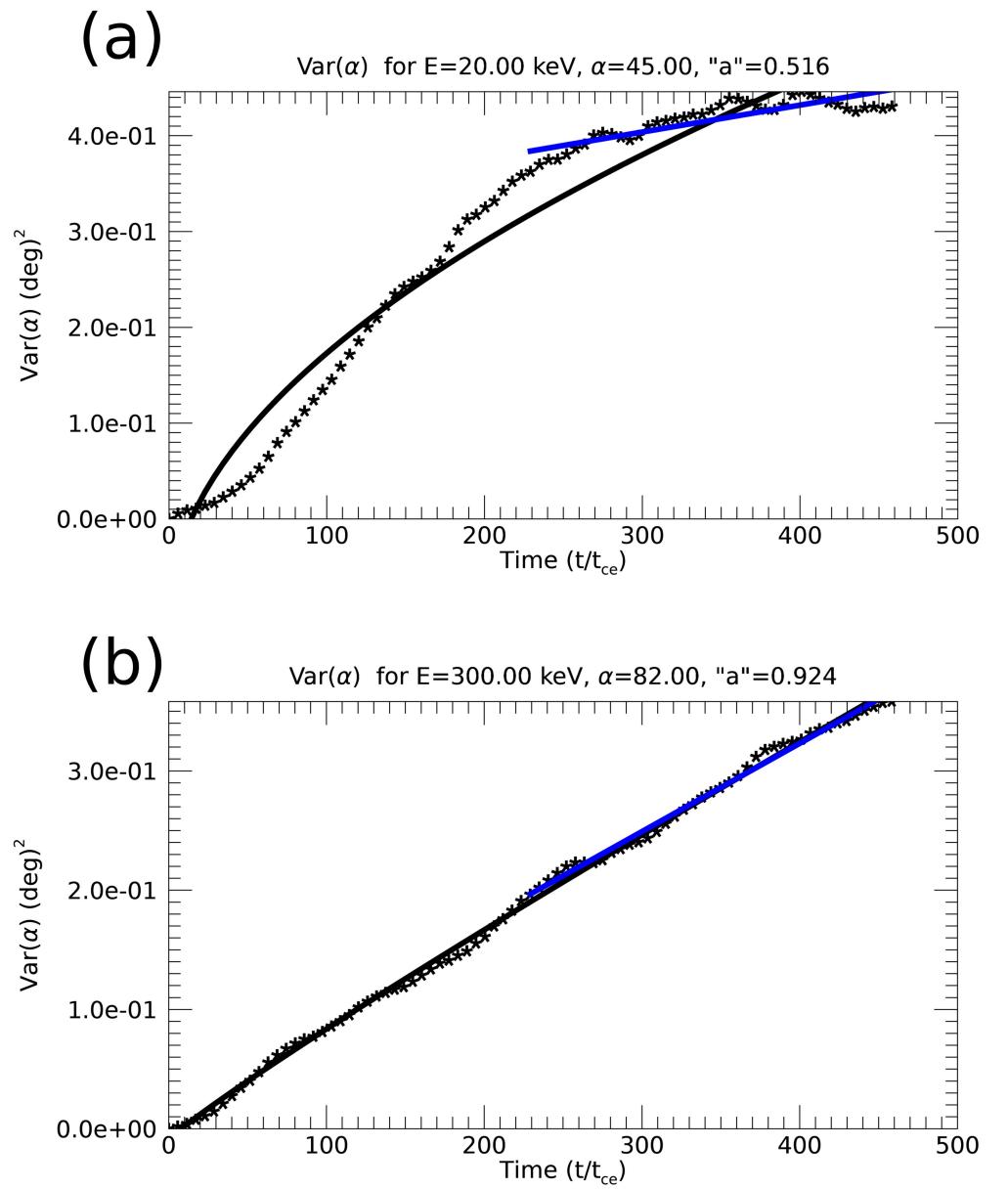


Figure 7.



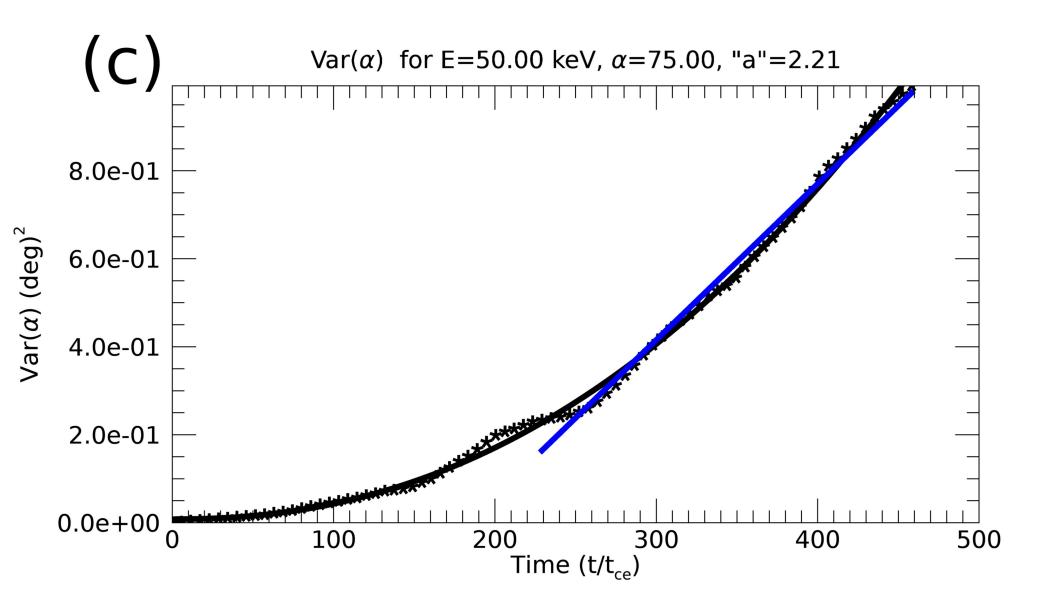


Figure 8.

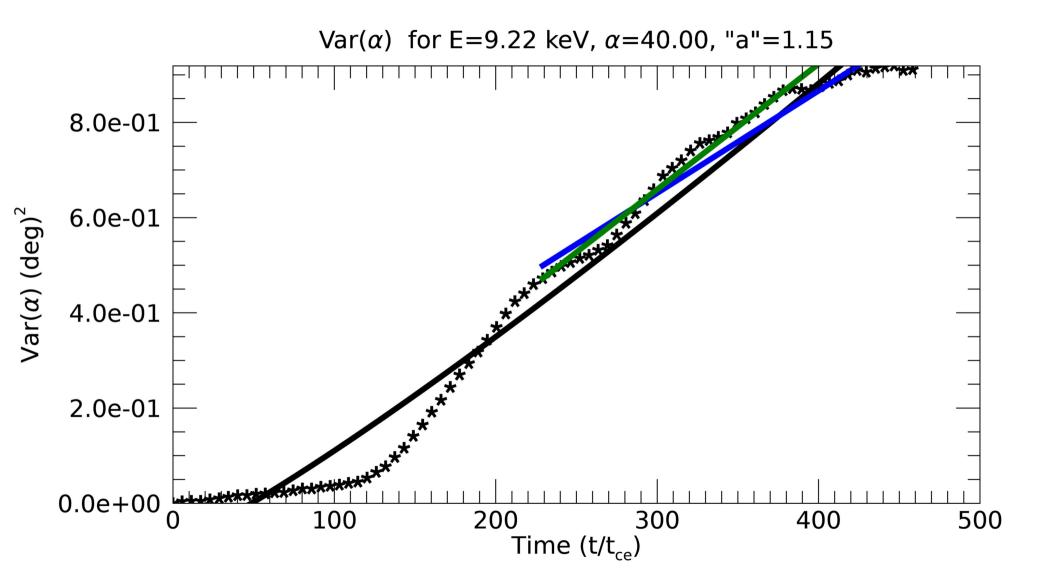
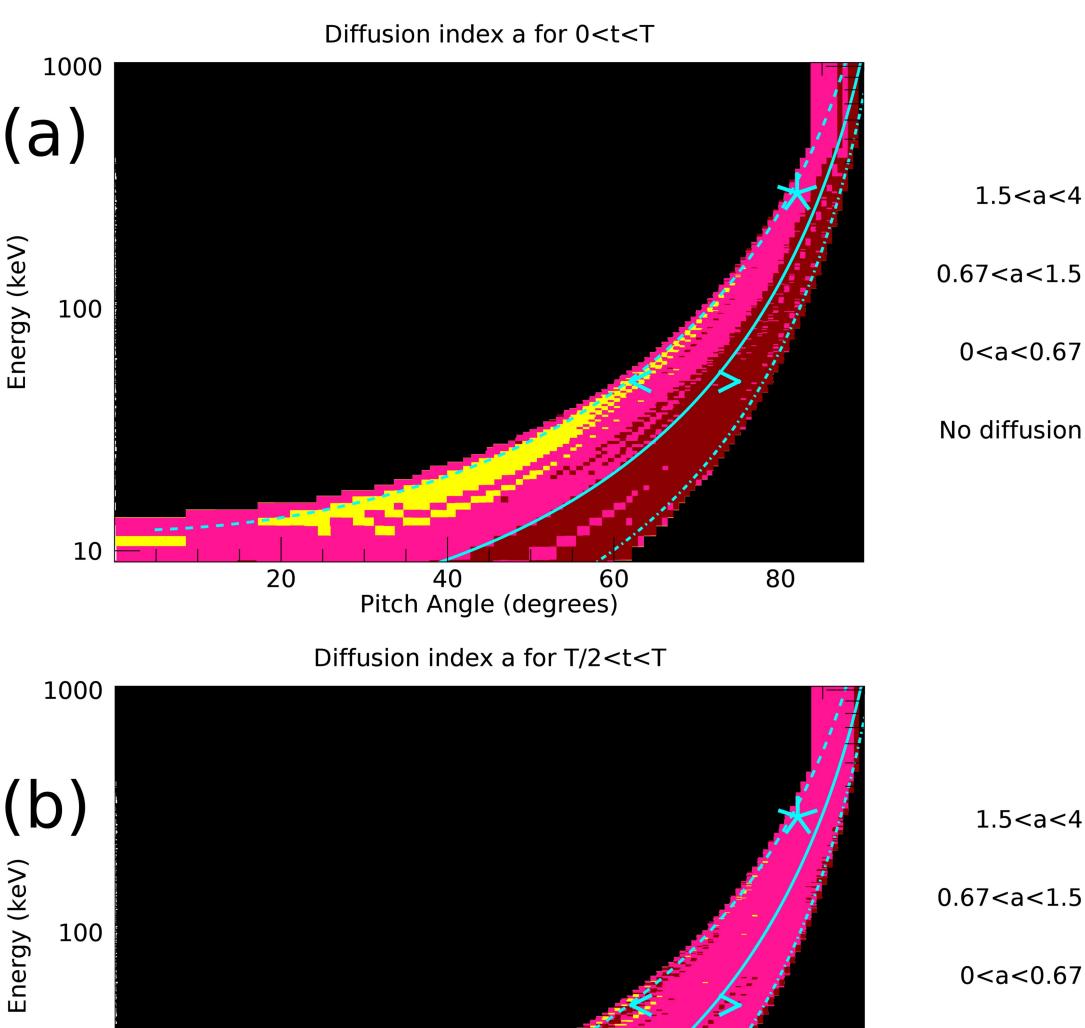


Figure 9.



Pitch Angle (degrees)

