Statistical analysis of fluctuations and noise-driven transport in particle-in-cell simulations of plasma turbulence

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The problem of discrete particle noise has been studied based on direct fluctuation measurements from gyrokinetic particle-in-cell simulations of stable plasmas. From the statistical analysis of electrostatic potential time evolution, the space-time correlation function has been measured. Fluctuation spectra have been constructed and analyzed in detail. Noise-driven transport is calculated using the quasilinear expression for the diffusion coefficient and the obtained noise spectrum. The theoretical value of electron heat conductivity shows good agreement with that measured in the simulation. It has been shown that for the realistic parameters in actual turbulence simulations, the noise-driven transport depends linearly on the entropy of the system. This study makes it possible to estimate and subtract the noise contribution to the total transport during turbulence simulations. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2673002]

I. INTRODUCTION

Gyrokinetic (GK) particle-in-cell (PIC) simulations have been widely used for studies of turbulent plasma since the first working code was demonstrated in 1983.[1] The advantage of the PIC method is its ability to describe systems with a large number of degrees of freedom[2] and its efficient use of state-of-the-art computational techniques.[3] Particle codes have been successfully applied for simulating drift wave turbulence such as ion temperature gradient (ITG)[4] and electron temperature gradient (ETG)[5] problems.

In PIC simulations, plasma is treated as a set of computational particles interacting with each other through self-consistently generated fields. The simulation algorithm can be divided into two major steps: first, calculation of fields based on a given particle distribution, and second, following the particle trajectories in these fields. The so-called "discrete particle noise" is produced at the first step when the distribution function and its moments are calculated using a relatively small number of computational particles ($N \sim 10^{10}$ in simulations versus $\sim 10^{23}$ in experiments). Considering these particles as Lagrangian markers carrying information about the distribution function, the problem of finding moments becomes equivalent to the evaluation of integrals in a large dimensional phase space using Monte-Carlo techniques.[6,7] Aiming to reduce the Monte-Carlo sampling noise, various approaches, such as the delta-f method,[8–10] have been developed. Another source of noise is the finite grid size in configuration space for PIC simulations, or in the phase space for continuum simulations.

Many studies have focused on the statistical properties of noise and its effect on simulated systems.[2,6,7,9–13] Treating the noise as a fluctuation of the distribution function, we come up with the Fokker-Planck (FP) collision integral describing diffusion in phase space.[14] In homogeneous systems, random fluctuations do not produce any net flux; however, in the case of drift wave turbulence, where background density and temperature gradients are present, the nonzero noise-driven flux must be taken into account. In addition to the generated flux, the small-scale noise could affect the dynamics of large-scale modes.[15]

The studies of GK noise are based on the general theory of electromagnetic fluctuations in stable plasmas.[16,17] Adopting the fluctuation-dissipation theorem (FDT),[11,12] the spectrum of the noise can be constructed and the coefficient of the associated diffusion can be found. These approaches, however, rely on the FDT, which is not strictly applicable in the case of turbulent plasmas far from thermodynamical equilibrium.[14,18] Some discussions on the theory of fluctuations in nonequilibrium systems, in particular using the general Klimontovich approach, can be found in Refs. 10 and 19.

The approach presented in this paper does not require theoretical calculations of noise spectra. Instead, the spectrum has been constructed using direct measurements of electrostatic fluctuations from simulation. Running the GK particle simulations with no instabilities, the only remaining transport would be due to the noise. We must keep the finite background temperature and density gradients in order to get nonzero flux, however these gradients must be small enough to prevent the development of drift instabilities. We use the values of gradients far below linear threshold, although one should be aware of the development of turbulence if approaching marginality.

As a result of the simulation, we can find the fluctuation correlation function and calculate the desired transport coefficient, which then can be compared with that directly measured in the simulation. Fluctuation spectra also provide us with additional information about the nature of the noise, which is important for understanding the effects of noise on the drift wave turbulence. This will be the subject of future work.

In Sec. II of this paper, we present simulation results for the electrostatic potential and give a detailed analysis of fluc-

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tuation spectra. In particular, it is shown that the fluctuation frequency spectrum is determined by the parallel wave vector and is practically independent of the perpendicular dynamics, which indicates that in our case the primary decorrelation mechanism is due to the parallel particle motion. Section III is devoted to calculation of the noise-driven transport based on the statistical properties of fluctuations. We demonstrate that for a wide range of noise levels, the heat conductivity depends linearly on the fluctuation intensity, which allows us to estimate the noise-driven transport using a simple scaling. The validity of the quasilinear expression for calculation of the diffusion coefficient, based on the known fluctuation spectrum, has been tested. The corresponding estimation of the electron heat conductivity shows good agreement with the simulation result. We also present direct measurements of noise-driven transport in simulations in the presence of ETG instabilities, which are compared with theoretical predictions based on linear scaling of transport with the particle weight square. This comparison shows very small differences between theory and measurements. The noise contribution in the simulation with 1000 particles per cell appears to be three orders of magnitude smaller than the total flux. Finally, the main conclusions of this paper are summarized in Sec. IV.

II. STATISTICAL PROPERTIES OF THE NOISE

Statistical properties of the noise were determined directly by processing the simulation data. The simulation was run with the gyrokinetic toroidal particle-in-cell code (GTC)[20] in a three-dimensional full torus. Toroidal geometry is treated rigorously using magnetic coordinates, which are desirable for global simulations.[3] In this electrostatic simulation, one species (ion or electron) is treated using the nonlinear GK method, and the other species (electron or ion) is assumed to be adiabatic. Thus the simulation here can be interpreted as the simulation of the ITG or ETG mode with subcritical background gradients. For convenience of notation, we use x for the radial direction, y for the poloidal direction, and z for the direction of the magnetic field line. The simulations have the following local electron parameters: $q=1.4$, $T_e/T_i=1$, $a/R_0=0.36$, and $\rho_e/R_0=0.358\times10^{-3}$. Here R_0 and a are the major and minor radii, T_e and T_i are the electron and ion temperatures, q is the safety factor, and ρ_e is the electron Larmor radius. The electron temperature and density scale lengths are set to be $R_0/L_T=1$ and $R_0/L_n=0.42$, which is far below the linear threshold for the ETG mode ($R_0/L_{T\text{threshold}}\approx4$). The number of grid points in the toroidal direction is $N_z=64$, in the radial direction $N_x=120$ and in the poloidal direction at the radial midpoint $N_y=2250$. The radial extension of the simulation domain is from $0.25a$ to $0.375a$. The number of particles per cell is two.

The initial random δf perturbations have been set up and evolve in time self-consistently using the nonlinear GK equation.[21] The value of the electrostatic potential was measured on a grid within the volume $L_x\times L_y\times L_z$, where $L_y=22\rho_e$, $L_x=24\rho_e$, and $L_z=(2/3)\pi R_0$. The diagnostic domain was located symmetrically with respect to the radial position at the center of the simulation domain and poloidal angle $\theta=\pi/2$. The data were collected over a period $T=350$ time steps, which is equal to 12.5 transit periods or, equivalently, to 4.5×10^4 gyroperiods.

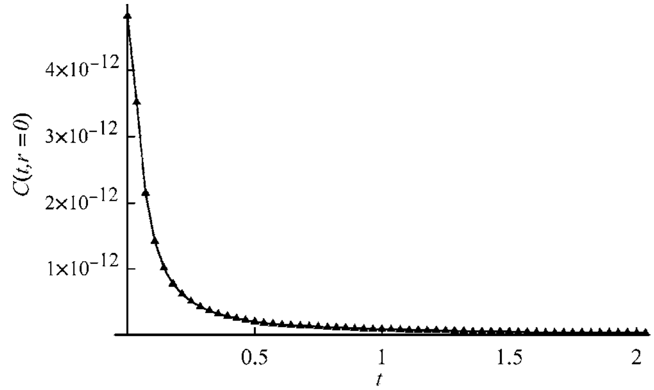

FIG. 1. Time correlation function of electrostatic potential, calculated at spatial displacement $\mathbf{r}=0$. Time separation is normalized by the transit period qR_0/v_e.

The fluctuation spectral density is defined as the Fourier-Laplace transform of the fluctuation correlation function

$$\langle|\Phi^2|\rangle_{\omega,\mathbf{k}}=\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}d\mathbf{r}\langle\Phi(t'+t,\mathbf{r}'+\mathbf{r})\Phi(t',\mathbf{r}')\rangle e^{-i\omega t+i\mathbf{k}\cdot\mathbf{r}}, \tag{1}$$

where the angular brackets mean statistical averages over the simulation domain, i.e., integration over t' and $\mathbf{r}'$.

The fluctuation correlation function $C(t,\mathbf{r})\equiv\langle\Phi(t'+t,\mathbf{r}'+\mathbf{r})\Phi(t',\mathbf{r}')\rangle$ obtained from the simulations is shown in Figs. 1–3. The one-point (spatial displacement $\mathbf{r}=0$) time dependence of the correlation function is presented in Fig. 1. As we can see, the characteristic time scale, defined as

$$\tau_c=\frac{\int tC(t,0)dt}{\int C(t,0)dt},$$

is of the order of $0.4T_{rt}$, where $T_{tr}=qR_0/v_e$ is the particle transit period. One-time spatial dependence in the perpendicular direction is plotted in Fig. 2. The signal correlation function looks slightly anisotropic in x and y, which could be explained by the presence of finite background gradients in

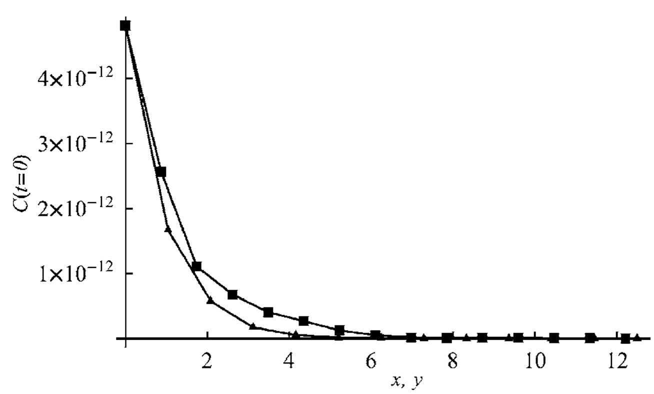

FIG. 2. Spatial correlation function of electrostatic potential in the radial (x, triangles) and poloidal (y, squares) directions. Spatial displacement is normalized by ρ_e.

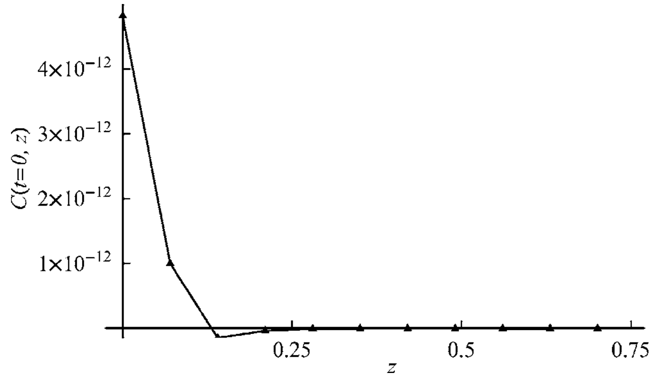

FIG. 3. Spatial correlation function of electrostatic potential in parallel direction. The displacement is normalized by qR_0.

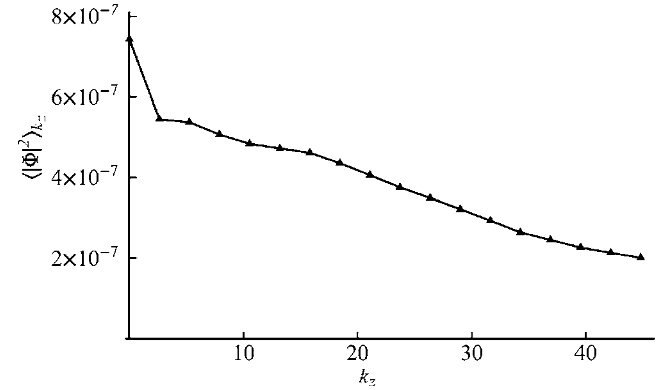

FIG. 5. The parallel wave-number dependence of fluctuation spectra. The parallel wave number is normalized by $1/qR_0$.

the x direction and the small ($\sim 10\%$) difference in grid size for these directions. The characteristic space scale in the perpendicular direction is of the order of one gyroradius. The correlation function dependence on parallel displacement is shown in Fig. 3. The parallel characteristic distance is $r_{c\parallel} \sim 0.03R_0$.

The fluctuation spectra calculated as a discrete Fourier transform of the fluctuation correlation function are shown in Figs. 4–7. The shapes of the perpendicular spectra (Fig. 4) are determined by a combination of the finite Larmor radius (FLR) effects and the numerical smoothing. On the other hand, the shape of the parallel spectrum (Fig. 5) is determined only by the numerical smoothing. Averaging in these figures has been done over frequencies and wave numbers other than those being plotted.

The frequency dependence is plotted for different values of the parallel (Fig. 6) and perpendicular (Fig. 7) wave numbers, averaged over the perpendicular and parallel wave numbers, respectively, and normalized by the root-mean-square value of the fluctuation intensity. It is clearly seen that the shape of the frequency spectra depends strongly on k_z and is practically independent of $k_\perp$. Moreover, it can be approximated by a Lorentzian form,[17,22]

$$f_L(\omega) = \frac{\omega_0}{\omega^2 + \omega_0^2}, \tag{2}$$

where the spectral width is determined with reasonable accuracy as $\omega_0 \approx k_z v_e$. This fact leads to the conclusion that the primary decorrelation mechanism is the parallel thermal motion. This is important for transport scaling and will be discussed in the next section.

III. CALCULATION OF TRANSPORT COEFFICIENTS

Considering the evolution of the guiding center distribution function in the presence of random electrostatic fluctuations, the Fokker-Planck type of equation can be written using derivations similar to those in Refs. 16 and 23. The FP collision integral would consist of several terms determined by the fluctuation correlation function. We restrict ourselves by taking into account only the term making a major contribution to the transport, namely the guiding center diffusion in configuration space. More sophisticated calculations might require considering other terms, in particular the friction term, as well.

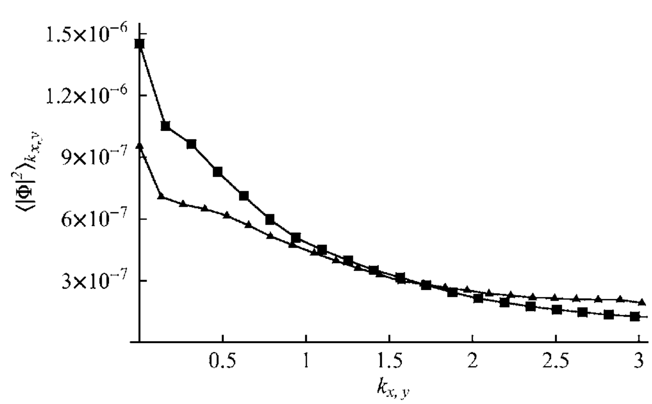

FIG. 4. The perpendicular wave-number dependence of fluctuation spectra (k_x, triangles; k_y, squares). Wave number is in units of $1/\rho_e$.

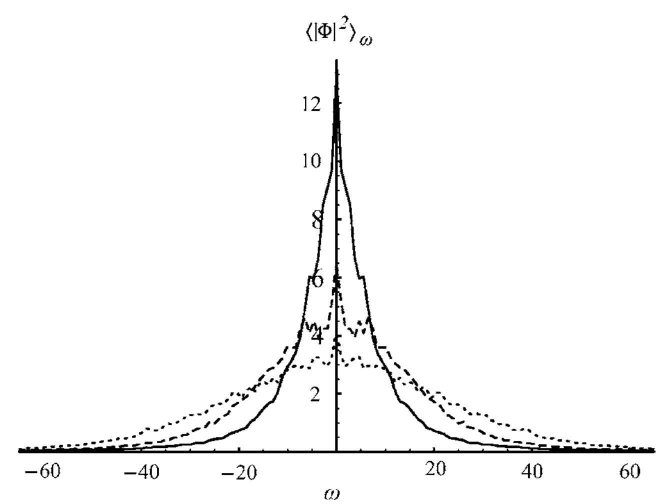

FIG. 6. Normalized frequency spectra for different values of parallel wave number. $k_z qR_0$=5.3 (solid line); 13.2 (dashed line); 21.1 (dotted line). The frequency is normalized by the inverse transit period v_e/qR_0.

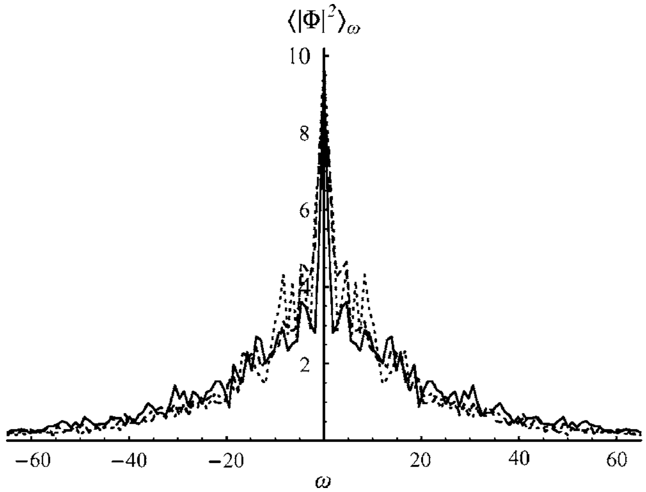

FIG. 7. Normalized frequency spectra for different values of perpendicular wave number. $k_\perp \rho_e = 0$ (solid line); 1.3 (dashed line); 2.6 (dotted line). The frequency is normalized by the inverse transit period v_e/qR_0.

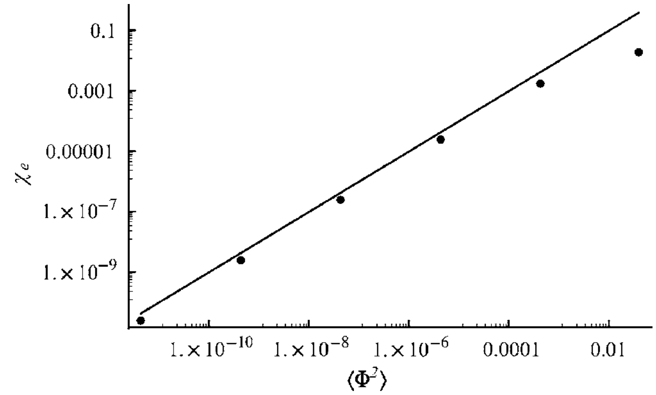

FIG. 8. Scaling of the electron thermal conductivity with fluctuation intensity. Here χ_e is in $v_e\rho_e$ units and electrostatic potential is normalized by T_e/e.

Following the transition probability formalism, the simple quasilinear expression for the mean-square displacement in the x direction of the test particle's guiding center under the influence of the fluctuating electrostatic field can be derived,[24]

$$\frac{\langle \Delta x^2 \rangle}{\tau} = \frac{2\pi c^2}{B^2 V} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \langle |\Phi^2| \rangle_{\omega,\mathbf{k}} k_y^2 J_0^2(k_\perp \rho_e)\, \delta(k_z v_z - \omega). \tag{3}$$

Here, the J_0 is the Bessel function of zeroth order, δ is the Dirac delta function, and V is the diagnostic volume. Equation (3) is written in the limit $\omega \ll \Omega_e$, and ignoring toroidal effects, since the obtained fluctuation characteristic frequency is $\omega_0/\Omega_e \sim 2\times 10^{-4}$ and $T_{tr} < \omega_d^{-1}$.

The spatial diffusion coefficient in the x direction is defined as

$$D(\mathbf{v}) = \frac{1}{2} \frac{\langle \Delta x^2 \rangle}{\tau}. \tag{4}$$

The dependence of the diffusion coefficient (4) on the parallel velocity appears through the frequency in the fluctuation correlation function, while the perpendicular velocity dependence is in the argument of the Bessel function, which is the FLR correction.

The form of the frequency dependence of the fluctuation spectrum is crucial in determining the diffusion coefficient. In fact, assuming, for example, a Lorentzian frequency dependence, the mean-square displacement can be found analytically and it would be inversely proportional to the width ω_0 of the Lorentzian spectrum (2). If this characteristic frequency would be determined by perpendicular motion characterized by the $v_{\mathbf{E}\times\mathbf{B}}$ velocity, the diffusion coefficient would be proportional to the amplitude of the fluctuations. Our measurements show that ω_0 depends on parallel motion, which is independent of the fluctuation amplitude, thus the mean-square displacement (3) must be proportional to the fluctuation intensity. To check this, we have varied the noise level in simulations by changing the value of the particle weight $w \equiv \delta f/f_0$, taking into account that the fluctuation amplitude is proportional to w. The results for the dependence of the heat conductivity on the noise intensity are shown in Fig. 8. As we can see, the linear scaling holds up to rms values of the fluctuation amplitude of order $e\Phi/T_e \sim 0.01$, which is much higher than a typical noise level in PIC simulations. At these values, the quantity $v_{E\times B}/r_{c\perp}$ becomes comparable to $v_e/r_{c\parallel}$ and thus parallel decorrelation is not dominant anymore.

The fact that noise-driven transport scales with the square of the particle weight[10] is important for estimating the noise contribution to the total flux in simulations of plasma turbulence. At the initial time, when no instabilities have developed, the proportionality coefficient c_0 between the particle weight w and the heat conductivity can be found,

$$\chi = c_0 w^2. \tag{5}$$

Assuming linear dependency and having the values of the particle weight available from simulations, we can estimate the noise contribution to the total flux at any time.

As an example, we consider a simulation of ETG turbulence that was run with GTC using 1000 particles per cell.[25] Direct measurements of the noise contribution to the flux can be done by the so-called scramble test. At a certain time moment, the toroidal positions of particles are randomized, keeping other parameters unchanged. This converts all ETG signals into noise and thus the obtained heat transport is purely the noise-driven one. The corresponding fluctuation intensity can be considered as the upper bound for the discrete particle noise level in the actual ETG simulation.

In Fig. 9, we plot the values of the noise-driven contribution to the electron heat conductivity estimated by the scramble test and by linear scaling (5). As we can see, the agreement between two curves is very good, which means that we can avoid doing costly scramble tests; instead, we can monitor the noise-driven input to the flux from the available simulation data for the particle weights, i.e., the entropy of the system. The values of electron heat conductivity measured in this GTC simulation show that the noise contribution is three orders of magnitude smaller than the total flux.

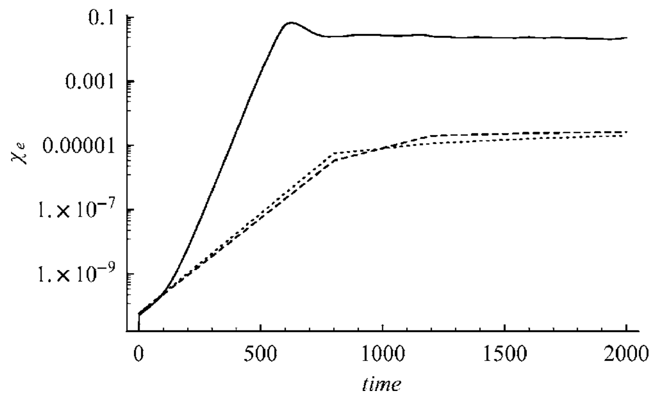

FIG. 9. Electron transport in ETG simulation: total (solid line), noise-driven contribution measured by scramble test (dashed line) and estimated from δf weight (dotted line). The electron heat conductivity is normalized by $v_e \rho_e$ and time is normalized by L_T / v_e.

Finally, we test the validity of the quasilinear expression (3) by comparing the electron heat conductivity based on this expression using fluctuation spectra presented in Sec. II with the value measured from simulations of random noise. We determine the heat conductivity as the heat flux divided by the temperature gradient $\chi_e = -q/(n \nabla T)$, where the heat flux can be written as

$$q = -\int d\mathbf{v} \frac{mv^2}{2} D(\mathbf{v}) \nabla f(\mathbf{v}) + \alpha T \int d\mathbf{v} D(\mathbf{v}) \nabla f(\mathbf{v}) = Q - \alpha T \Gamma. \tag{6}$$

Here f is the Maxwellian velocity distribution with temperature and density gradients in the x direction. The last term in (6) is the contribution from the particle flux. It vanishes in the simulation due to the quasineutrality condition, and thus must be subtracted in the quasilinear calculations. The coefficient $\alpha \sim 1$ is found by considering the case with no temperature gradient but finite density gradient, such that $q=0$ and $\alpha = Q/T\Gamma$. The value of the electron thermal conductivity calculated using Eqs. (3)–(6) is $\chi_{eql} = 4.18 \times 10^{-11}$ in $\rho_e v_e$ units, and the corresponding value obtained from simulation is $\chi_{e\ \mathrm{sim}} = (2.41 \pm 0.35) \times 10^{-11}$. As we can see, the theory prediction is somewhat overestimated. A possible reason for that is that we neglect the friction term in the FP collision operator. This is equivalent to the difference between the self-consistent heat flux calculated in the simulations as $Q_{\mathrm{sim}} = \int \frac{1}{2} mv^2 \delta v_{E\times B} \delta f d\mathbf{v}$ and the heat flux based on the random-walk model $Q = -\int \frac{1}{2} mv^2 D(\mathbf{v}) \nabla f(\mathbf{v}) d\mathbf{v}$. This problem is discussed for the ITG case in Ref. 26, and it will be studied further in our future research.

IV. SUMMARY AND DISCUSSION

We have done a detailed analysis of electrostatic fluctuation data obtained from gyrokinetic PIC simulations in the absence of drift instabilities. From the obtained noise spectrum, we draw the conclusion that the primary decorrelation mechanism is particle parallel motion, having a different time scale compared to the plasma collective effects. Careful studies, however, must be done on the problem of the interplay between noise and plasma turbulence, when the pressure gradient is close to or above the instability threshold, which is beyond the scope of this paper and could be the subject of future work.

We have found that noise-driven transport scales linearly with the fluctuation intensity. This means that in turbulence simulations, the contribution to transport due to the discrete particle noise, typically a few orders of magnitude smaller than the total flux, can be estimated with reasonable accuracy either by direct measurements or based on the value of the particle weights, using the linear scaling. Also we have shown that the quasilinear expression for the diffusion coefficient, based on the obtained fluctuation spectrum, gives a value of the heat conductivity that is in rather good agreement with the one measured directly.

This study finds that in the δf simulation on the turbulence time scale, the turbulent transport can reach a quasi-steady state before the particle noise grows to a high level to affect the turbulence. It addresses some of the recent concerns about the credibility of the PIC approach for the simulations of turbulent saturated states. Further extension of the applicability regime, in order to treat transport time scales, would require, however, using the full-f or revised δf method.

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