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Nonequilibrium Gyrokinetic Fluctuation Theory and Sampling Noise in Gyrokinetic Particle-in-cell Simulations

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Nonequilibrium gyrokinetic fluctuation theory and sampling noise in gyrokinetic particle-in-cell simulations

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The present state of the theory of fluctuations in gyrokinetic (GK) plasmas and especially its application to sampling noise in GK particle-in-cell (PIC) simulations is reviewed. Topics addressed include the Δf method, the fluctuation-dissipation theorem for both classical and GK many-body plasmas, the Klimontovich formalism, sampling noise in PIC simulations, statistical closure for partial differential equations, the theoretical foundations of spectral balance in the presence of arbitrary noise sources, and the derivation of Kadomtsev-type equations from the general formalism. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2759879]

I. INTRODUCTION

Recently Nevins *et al.*[1] argued that sampling noise in the gyrokinetic (GK) particle-in-cell (PIC) simulation technique can be problematical in certain cases. Although they did not claim that all GK-PIC simulations are noise-dominated and they specifically published other adequately converged runs,[2,3] various questions have been raised about their methodology. It is understandable that a certain amount of confusion or misunderstanding has occurred because estimates of noise require subtle considerations of nonlinear statistical dynamics. Nevertheless, there is an underlying systematology. Since the theory used by Nevins *et al.* was based on earlier calculations by the present author[4,5] (extended by Nevins *et al.* to account for certain numerical details such as an adiabatic species and finite-sized particles), it seems timely to review the foundations. Specifically, I shall focus on the applicability of the fluctuation-dissipation theorem (FDT) and the form of the nonequilibrium spectral balance equation in the presence of both self-consistently generated turbulence and algorithmically induced sampling error. No attempt is made to describe physics results from simulations or to survey analytical descriptions of specific instances of microturbulence; I am concerned here with the basic theory of fluctuations. An initial account of this work was given in Ref. 6. Another review article that may provide useful background on statistical turbulence theory is Ref. 7.

A. Introductory remarks on noise, gyrokinetics, and the Δf simulation algorithm

The importance of noise in physical systems has been recognized for more than a century. A large amount of literature going back to Gibbs and Boltzmann[8] on the statistical-mechanical description of the many-body problem cannot be cited here. Einstein's insights (circa 1905) into Brownian motion[9,10] are well known. G. I. Taylor investigated turbulent eddy motion in the atmosphere as early as 1915 (Ref. 11) and published a fundamental paper on Brownian motion in fluid turbulence a few years later.[12] Plasma physicists are well schooled in the kinetic-theoretical derivations of the plasma collision operator,[13] with the Klimontovich formalism[14] being preferred for both its technical simplicity and physical appeal.

The Klimontovich equation (see Sec. III B) contains all physics of the N-body problem, but if solved rigorously presents a difficult computational problem of $O(N^2)$ and contains substantial noise at short scales due to close encounters. In the PIC method,[15,16] the Coulomb interaction is regularized at short distances (equivalent to considering a charge cloud of nonzero size) in order to reduce the short-wavelength (collisional) noise, and collective fields are calculated from the charge distribution of particles deposited on a spatial grid. The effect is to provide an $O(N)$ integration of the (collisionless) Vlasov equation. Of course, that equation can be attacked by more conventional numerical methods as well.

The Vlasov equation is a continuous partial differential equation (PDE). As such, it exhibits no discreteness-related noise. However, the PIC method, being built on a collection of discrete particles (interacting through collective fields), does exhibit such noise. Morse and Nielson[17] described the "full-f" PIC method by saying, "The electrons are represented by a number… of appropriately weighted simulation particles which are initially distributed uniformly in x and randomly in v… and which may be thought of as *random Lagrangian mesh points imbedded in a collisionless phase fluid rather than as very large real particles.*" Birdsall and Langdon[15,18] called the particles *Lagrangian markers*, and emphasized that because their number is finite a kind of Monte Carlo sampling noise is introduced into the simulation. Analytical calculations of that noise (including the effects of finite-sized particles) were reported by Langdon and Birdsall,[16] who also cited successful numerical tests of the analytical formula [Eqs. (26a) and (26b)]. Use of the FDT for such calculations was described by Langdon[18] and Birdsall and Langdon.[15]

With the development of nonlinear gyrokinetics[19–21] and the advent of GK particle simulation[20] in the early 1980s, it

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became necessary to extend noise calculations to the GK context. Krommes's calculations of GK noise in plasmas consisting of discrete gyrocenters[4,22,23] will be described in Sec. III. A distinct problem is posed by the Δf-PIC algorithm[24–27] for solving the GK equation (GKE). That is also a smooth PDE. However, when PIC methods are used to solve the equation, Monte Carlo sampling again leads to noise quite similar to the discreteness effects that arise in many-body plasmas. This was clarified by Aydemir[28] and Hu and Krommes.[5] The latter authors also performed a Klimontovich-based analytical calculation of Δf sampling noise.

In the Δf method, the distribution function f is written as an analytically known reference distribution f_0 plus a correction[29] Δf: $f=f_0+\Delta f$, and only Δf is solved for numerically. (In practice, a dimensionless "particle weight" w is evolved, as will be described below.) In a PIC algorithm, the Δf decomposition obviates the need to sample f_0, thereby substantially reducing the sampling noise for a given number of samples.[30] Unfortunately, in strictly collisionless simulations a fundamental difficulty emerges: The mean-square weight $W \doteq \langle w^2 \rangle$ (I use $\doteq$ for definitions) grows indefinitely with time[31] (for fixed background gradient).[32] Krommes and Hu[33] called this phenomenon the *entropy paradox*, since it is impossible to achieve a truly steady-state simulation in the face of an evolving $\langle w^2 \rangle$, yet "steady-state" fluxes of particles and heat were routinely quoted from such simulations. Krommes and Hu argued (and demonstrated with examples) that a small amount of collisional dissipation would resolve the paradox, since that dissipation may remain nonzero even as the limit of zero collisionality is approached. Steady-state entropy balances have been subsequently verified numerically by[34] Watanabe and Sugama[35] and Candy and Waltz.[36]

Simple estimates[25,28] (refined by Hu and Krommes[5]) and simulations show that the intensity of sampling noise scales with W. It is thus clear that simulations in which W grows indefinitely[37] will have problems with signal-to-noise ratio at long times; the only questions are the size of the effect and whether one can extract useful information at intermediate times, before the signal is either swamped or eliminated[38] by the sampling noise. Nevins *et al.* made detailed calculations of sampling noise that agreed very well with simulations. In spite of that agreement, however, their results (which showed that certain simulations could be noise-dominated) were questioned on the grounds that formulas derived for near-thermal equilibrium were unjustifiably applied to a turbulent, nonequilibrium regime. That brings us to the fundamental question addressed in this review: *What are the structure and implications of the nonequilibrium spectral balance equation in the presence of both self-consistent turbulence and sampling noise?* In order to answer it, I shall provide an introductory tour through statistical fluctuation theory, including its relatively recent applications to gyrokinetics.

It is, of course, of great interest to develop numerical algorithms that cure the problem of growing weights, and various approaches have been suggested.[39–42] Although a review of modern simulation methodology would be very useful, the length constraint precludes such a discussion here. Instead, I focus on theoretical techniques relating to the calculation of statistical noise.

B. Spectral balance: Basic concepts

Before delving into systematic formalism, I shall give a brief and nonrigorous introduction to some important issues relating to spectral balance, beginning with basic definitions. Assume that the turbulent fluctuations are statistically homogeneous (at least locally). Let $C_{\boldsymbol{k}}(t,t')$ be the two-time correlation function of fluctuations $\delta\psi_{\boldsymbol{k}}$ of a Fourier amplitude $\psi_{\boldsymbol{k}}$ such as the electrostatic potential $\phi_{\boldsymbol{k}}$: $C_{\boldsymbol{k}}(t,t') = \langle \delta\psi_{\boldsymbol{k}}(t)\delta\psi^*_{\boldsymbol{k}}(t')\rangle \equiv C_{\boldsymbol{k}}(\tau|T)$, where $\tau \doteq t-t'$ and $T \doteq \frac{1}{2}(t+t')$. ($\psi_{\boldsymbol{k}}$ might be a distribution function, in which case it would depend on velocity. I do not indicate that detail in this section.) The wave-number spectrum is then $C_{\boldsymbol{k}}(t) \equiv C_{\boldsymbol{k}}(t,t) = C_{\boldsymbol{k}}(0|t)$. In a statistically steady state, $C_{\boldsymbol{k}}(t)$ is independent of t and $C_{\boldsymbol{k}}(t,t')=C_{\boldsymbol{k}}(\tau)$.[43] More generally, one may assume that $C_{\boldsymbol{k}}(\tau|T)$ depends weakly on T; I usually do not indicate that dependence explicitly. Because of turbulent mixing, one expects that $C_{\boldsymbol{k}}(\tau)$ should fall rapidly to zero as $|\tau| \to \infty$. Thus one assumes that $C_{\boldsymbol{k}}(\tau)$ is integrable. This guarantees that the temporal Fourier transform exists and permits introduction of the frequency spectrum, $C_{\boldsymbol{k}}(\omega) \doteq \int_{-\infty}^{\infty} d\tau\, e^{i\omega\tau} C_{\boldsymbol{k}}(\tau)$ [thus $C_{\boldsymbol{k}}(t) = (2\pi)^{-1}\int_{-\infty}^{\infty} d\omega\, C_{\boldsymbol{k}}(\omega)$]. The requirement that the time-lagged correlation function decays at $\pm\infty$ precludes singularities of $C_{\boldsymbol{k}}(\omega)$ on the real frequency axis, i.e., contributions of the form $\delta(\omega)$ or $\delta(\omega - \Omega_{\boldsymbol{k}})$.

The level of fluctuations at a specified $\boldsymbol{k}$ and ω is set by a competition between forcing and damping. The equation that determines the result of that competition is called the *spectral balance equation*. In steady state, one way of expressing it (for more discussion, see Sec. IV) is

$$C_{\boldsymbol{k}}(\omega) = R_{\boldsymbol{k}}(\omega) F_{\boldsymbol{k}}(\omega) R^*_{\boldsymbol{k}}(\omega), \tag{1}$$

where the forcing function $F_{\boldsymbol{k}}$ is the covariance of "incoherent" or "bare" fluctuations and the response or damping function $R_{\boldsymbol{k}}$ will be discussed in more detail shortly. Fundamental discussion on the interpretation of Eq. (1) was given by Kraichnan[44] in the context of his direct-interaction approximation (DIA). $R^{-1}_{\boldsymbol{k}}$ is closely related to the dielectric function $\mathcal{D}(\boldsymbol{k},\omega)$.[45] For the present qualitative discussion it is adequate to write

$$C_{\boldsymbol{k}}(\omega) = \frac{N_{\boldsymbol{k}}(\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2}, \tag{2}$$

where $N_{\boldsymbol{k}}(\omega) \propto F_{\boldsymbol{k}}(\omega)$. Thus an interpretation of Eq. (1) is that the dielectric properties of the turbulent medium shield bare fluctuations, giving rise to the observable spectrum. This concept is well known in the context of test-particle methods in elementary plasma kinetic theory,[46] where $N_{\boldsymbol{k}}$ is related to the Cerenkov emission, but it also applies to turbulent situations. The distinction is that whereas the point structure and free-streaming motion of a test particle are known, in turbulence the bare fluctuations arise from various nonlinear processes that must be determined self-consistently.

Because $C_{\boldsymbol{k}}(\tau)$ decays at infinity, one deduces that $\mathcal{D}(\boldsymbol{k},\omega)$ has no zeros on the real ω axis; the assumptions of steady state and causality preclude zeros in the upper half of the ω plane. Thus all collective modes should be damped, not marginally stable. Jenkins and Lee[47] have studied a model in which modes approach marginal stability as the nonlinearities saturate. Although instructive, such models do not capture some important characteristics of a truly turbulent steady state, so should be viewed with caution.

"Forcing" in this context should not be confused with linear instability; we shall see that the usual linear growth rate $\gamma_{\boldsymbol{k}}$ is contained in $R_{\boldsymbol{k}}$ (as a negative damping). The forcing effects contained in the numerator of Eq. (2) can arise from either (i) direct external random forcing, in which case $F_{\boldsymbol{k}}(\tau)$ is the covariance of that forcing; (ii) particle discreteness effects (which are a special kind of "external" forcing because the point structure of a particle is not modified by the turbulence); (iii) the nonlinear beating of fluctuations at other wave numbers ($\boldsymbol{p}$ and $\boldsymbol{q}$) and frequencies (ω' and ω'');[48] or (iv) additional sources of noise such as Monte Carlo sampling error.[5,28] Discussion of the role and calculation of sampling error is the ultimate goal of this article.

The total damping arises from both linear response and turbulent mixing (which may also include effects due to discrete particles and sampling errors). A basic model for $R_{\boldsymbol{k}}$ includes a linear frequency $\Omega_{\boldsymbol{k}}$, a linear growth rate $\gamma_{\boldsymbol{k}}$, and a nonlinear "coherent" (possibly complex) damping rate $\eta_{\boldsymbol{k}}^{\mathrm{nl}}$:

$$\partial_t R_{\boldsymbol{k}}(t;t') + (i\Omega - \gamma_{\boldsymbol{k}})R_{\boldsymbol{k}} + \eta_{\boldsymbol{k}}^{\mathrm{nl}} R_{\boldsymbol{k}} = \delta(t-t'). \tag{3}$$

Thus in steady state ($\eta_{\boldsymbol{k}}^{\mathrm{nl}}$ constant in time) $R_{\boldsymbol{k}}(\omega)=[-i(\omega+i\eta_{\boldsymbol{k}})]^{-1}$, where $\eta_{\boldsymbol{k}} \doteq \mathrm{Re}\,\eta_{\boldsymbol{k}}^{\mathrm{nl}} - \gamma_{\boldsymbol{k}} + i(\Omega_{\boldsymbol{k}} + \mathrm{Im}\ \eta_{\boldsymbol{k}}^{\mathrm{nl}})$. One sees that nonlinearity works to defeat linear growth; it can also give rise to a frequency shift. Turbulent line broadening arises from $\mathrm{Re}\ \eta_{\boldsymbol{k}} = \mathrm{Re}\ \eta_{\boldsymbol{k}}^{\mathrm{nl}} - \gamma_{\boldsymbol{k}}$.

$R_{\boldsymbol{k}}(\tau)$ is related to the transient response of the turbulent system to small perturbations. A spatially homogeneous system subjected to a statistically sharp forcing $\hat{f}_{\boldsymbol{k}}(t)$ will exhibit a causal response $\Delta\tilde{\psi}_{\boldsymbol{k}}(t) = O(\hat{f}_{\boldsymbol{k}})$. That response is random (indicated by the tilde), reflecting the nonlinear stochastic properties of the background turbulence. On the average, one has

$$\langle \Delta\psi_{\boldsymbol{k}}(t)\rangle = \int_{-\infty}^{t} dt'\, R_{\boldsymbol{k}}^{(1)}(t;t')\hat{f}_{\boldsymbol{k}}(t') + \frac{1}{2}\int_{-\infty}^{t} dt'\, dt'' \sum_{\Delta} R_{\boldsymbol{p},\boldsymbol{q}}^{(2)*}(t;t',t'')\hat{f}_{\boldsymbol{p}}^{*}(t')\hat{f}_{\boldsymbol{q}}^{*}(t'') + \cdots , \tag{4}$$

where Σ_{Δ} signifies the sum over all wave-number triads such that $\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q}=\boldsymbol{0}$.[49] This expansion defines a series of Taylor coefficients or response functions $R^{(n)}$. The first-order coefficient, which describes the response to a sharp impulse, is called the *infinitesimal response function*; it is the same R encountered in Eq. (1): $R_{\boldsymbol{k}} \equiv R_{\boldsymbol{k}}^{(1)}$. (This clarifies why R and $\mathcal{D}^{-1}$ are intimately related.) In steady state, causality guarantees that $R_{\boldsymbol{k}}(\tau) \propto H(\tau)$, where $H(\tau)$ is the unit step function. One expects that turbulent mixing causes $R_{\boldsymbol{k}}(\tau)$ to decay as $\tau \to \infty$. For that to be true, one must have $\mathrm{Re}\ \eta_{\boldsymbol{k}}^{\mathrm{nl}} > \gamma_{\boldsymbol{k}}$.[50] This ensures that $R_{\boldsymbol{k}}(\omega)$ is analytic in the upper half-plane.

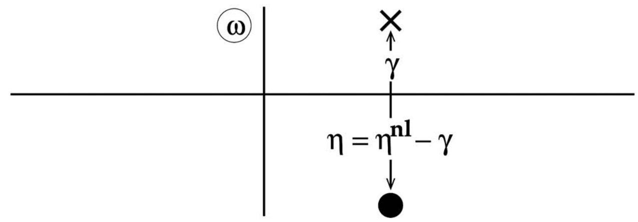

FIG. 1. Zeros of the steady-state dielectric function $\mathcal{D}(\boldsymbol{k},\omega)$ for turbulence always lie in the lower, stable half of the frequency plane (filled circle), even though zeros of the linear approximation $\mathcal{D}^{(0)}(\boldsymbol{k},\omega)$ lie in the upper half-plane for linearly unstable modes (cross). Nonequilibrium spectral balance must be formulated in terms of $\mathcal{D}$, not $\mathcal{D}^{(0)}$. For a given wave number, the nonlinear damping $\eta_{\boldsymbol{k}}^{\mathrm{nl}}$ is always greater than the linear growth rate $\gamma_{\boldsymbol{k}}$.

It is crucially important to distinguish between the "linear" dielectric function $\mathcal{D}^{(0)}$ and the fully nonlinear dielectric $\mathcal{D}$.[7] This distinction may be confusing because $\mathcal{D}^{-1}$ is an infinitesimal response function that describes first-order response to external forcing; thus one might ask, Why are not all dielectrics "linear"? The well-known answer is that linearity is with respect to the forcing, not the background turbulence. The properties of that turbulence can be fully described only by terms through all orders in the nonlinear coupling. By definition, the linear dielectric $\mathcal{D}^{(0)}$ ignores the nonlinearity altogether. It is very difficult to fully determine the complete $\mathcal{D}$, but its basic properties can be understood by referring to the model (3) for $R_{\boldsymbol{k}}(\tau)$. Since $\mathrm{Re}\ \eta_{\boldsymbol{k}}^{\mathrm{nl}} > \gamma_{\boldsymbol{k}}$, one sees that the zero of $\mathcal{D}(\boldsymbol{k},\omega) \propto R_{\boldsymbol{k}}^{-1}(\omega)$ indeed lies in the lower half of the ω plane even though for linear instability ($\gamma_{\boldsymbol{k}} > 0$) the zero of $\mathcal{D}^{(0)}$ is in the upper half-plane (see Fig. 1).

So far I have focused on the discussion about nonlinear damping on frequency-dependent dielectric response, a topic familiar to plasma physicists. But there is a simpler way of understanding the essence of spectral balance that proceeds from the time-dependent equation for a nonstationary $C_{\boldsymbol{k}}(t)$. One has $\partial_t C_{\boldsymbol{k}}(t,t) = [\partial_t C_{\boldsymbol{k}}(t,t') + \partial_t C_{\boldsymbol{k}}(t',t)]_{t'=t} = 2\,\mathrm{Re}[\partial_t C_{\boldsymbol{k}}(t,t')]_{t'=t}$. The last derivative can be evaluated from the two-time spectral balance [the inverse Fourier transform of Eq. (1)] written in the form $R^{-1}C(t,t') = \int_{-\infty}^{t'} d\bar{t}\, F_{\boldsymbol{k}}(t,\bar{t}) R_{\boldsymbol{k}}^{*}(t';\bar{t})$. If one idealizes $F_{\boldsymbol{k}}(t,t')$ as white noise, i.e., $F_{\boldsymbol{k}}(t,t') = 2F_{\boldsymbol{k}}\delta(t-t')$ ($F_{\boldsymbol{k}} > 0$), the final result is

$$\partial_t C_{\boldsymbol{k}}(t) = 2\gamma_{\boldsymbol{k}} C_{\boldsymbol{k}} - 2\ \mathrm{Re}\ \eta_{\boldsymbol{k}}^{\mathrm{nl}} C_{\boldsymbol{k}} + 2F_{\boldsymbol{k}}. \tag{5}$$

In steady state, this reduces to the balance[51]

$$\underbrace{\mathrm{Re}\ \eta_{\boldsymbol{k}}^{\mathrm{nl}}}_{\substack{\text{coherent}\\ \text{nl damping}}} = \underbrace{\gamma_{\boldsymbol{k}}}_{\substack{\text{linear}\\ \text{growth}}} + \underbrace{F_{\boldsymbol{k}}/C_{\boldsymbol{k}}}_{\substack{\text{incoherent}\\ \text{forcing}}} . \tag{6}$$

Because $F_{\boldsymbol{k}}$ (a positive-definite variance) and $C_{\boldsymbol{k}}$ are positive, one sees that the nonlinear damping rate must inevitably be larger than the linear growth rate if incoherent forcing exists at all. That is virtually always the case in realistic situations, so models that ignore incoherent forcing must be viewed skeptically.

C. Outline of the article

Given the spectral function $C_{\boldsymbol{k}}$, one can calculate transport coefficients or fluxes. (In detail, one requires cross correlations if ψ is a fluid variable; the present terse notation does not distinguish the possibly tensor character of C.) A basic goal is to assess how the spectral level (and thus the size of the transport coefficients) depends on various effects such as an increase in sampling error. Naively, one might think that more noise would imply more total transport, but that does not necessarily follow because the spectral balance equation is in general highly nonlinear (both η^{nl} and F are functionals of R and C) and assessing the result of the balance between nonlinear forcing and nonlinear damping (in the face of energy conservation for the nonlinear contributions to the wave-number-integrated spectrum) is nontrivial. In the remainder of the article I shall address various facets of such analysis. In Sec. II I describe the Δf algorithm in the context of PIC simulation. In Sec. III I briefly review classical results on discreteness-induced fluctuations. In Sec. IV I touch on the opposite extreme of fluctuations in continuous PDEs with smooth initial conditions; that gives rise to classical statistical turbulence theory.[52] In Sec. V I mention the beautiful formalism of Rose[53] that allows discrete and continuous effects to be treated on equal footing. I also show how to derive from the general structure the simple model spectral balance equation discussed by Kadomtsev,[54] the proper interpretation of which has generated some controversy. (I propose a minor variant of that equation, but its essential content is preserved.) In Sec. IV I attempt to apply the general results to the Δf-PIC problem. Although certain technical details have not been fully analyzed at this point, the broad outline of the theory is clear and would appear to support the basic analyses by Nevins *et al.* I review the various issues and results in Sec. VII. (It would likely be useful for the reader to peruse that discussion now before tackling the detailed mathematics to follow.) Several appendices complete the article.

II. THE Δf EQUATIONS AND PIC SIMULATION

Let us assume that we are to solve the collisionless kinetic equation

$$\partial_t f(z,t) - \hat{L} f + \partial_z \cdot (V[f] f) = 0. \tag{7}$$

Here z is the collection of independent variables (e.g., $\{\boldsymbol{R}, \mu, v_\parallel\}$ in gyrokinetics, where $\boldsymbol{R}$ is the gyrocenter position, μ is the magnetic moment, and $v_\parallel$ is the velocity parallel to the magnetic field), $\hat{L}$ is a linear operator (e.g., $\hat{L} = -v_\parallel \nabla_\parallel$), brackets denote functional dependence, and $\boldsymbol{V}[f]$ is a linear functional of f (so the product $V[f]f$ describes a quadratic nonlinearity). The GK-Poisson system can be written in this form with $\boldsymbol{V} = (\bar{\boldsymbol{V}}_E, qE_\parallel/m)$ and[55] $\partial_z = (\boldsymbol{\nabla}_\perp, \partial_{v_\parallel})$. Covariant notation is sometimes useful,[56] but is unnecessary here.

A. Δf versus δf

In the Δf method, one writes[29]

$$f = f_0 + \Delta f, \quad \boldsymbol{V} = \boldsymbol{V}_0 + \Delta \boldsymbol{V}, \tag{8}$$

where f_0 is an arbitrary reference distribution that is assumed to be known and to obey

$$(\partial_t - \hat{L}) f_0 + \partial_z \cdot (\boldsymbol{V}_0[f_0] f_0) = -S, \tag{9}$$

thus defining the sink function S. [It is frequently assumed that f_0 satisfies the kinetic equation (7), in which case S vanishes.] One readily finds

$$(\partial_t - \hat{L}) \Delta f + \partial_z \cdot (\boldsymbol{V}_0 \Delta f) + \partial_z \cdot (\Delta \boldsymbol{V} f_0) + \partial_z \cdot (\Delta \boldsymbol{V} \Delta f) = S. \tag{10}$$

I shall call Eq. (10) the "Δf equation"; it is the fundamental PDE that is to be solved. Before discussing in Sec. II B the PIC method for its approximate numerical solution, let me contrast Eqs. (9) and (10) with the closely related equations used in the statistical theory of turbulence.[7] There f is treated as a random variable[57] and decomposed into its mean and fluctuating parts:

$$f = \langle f \rangle + \delta f. \tag{11}$$

The mean field obeys

$$(\partial_t - \hat{L}) \langle f \rangle + \partial_z \cdot (\langle \boldsymbol{V} \rangle \langle f \rangle) + \partial_z \cdot \langle \delta \boldsymbol{V} \delta f \rangle = 0, \tag{12}$$

and subtracting this from Eq. (7) yields

$$\begin{aligned}(\partial_t - \hat{L}) \delta f &+ \partial_z \cdot (\langle \boldsymbol{V} \rangle \delta f) + \partial_z \cdot (\delta \boldsymbol{V} \langle f \rangle) \\ &+ \partial_z \cdot (\delta \boldsymbol{V} \delta f - \langle \delta \boldsymbol{V} \delta f \rangle) = 0.\end{aligned} \tag{13}$$

The role of the $\langle \delta \boldsymbol{V} \delta f \rangle$ term in Eq. (13) is to ensure that Eq. (13) maintains the exact result $\langle \delta f \rangle = 0$, which is a basic consequence of the decomposition (11). I shall call Eq. (13) the "δf equation."

If one compares Eq. (9) with Eq. (12) and also compares Eq. (10) with Eq. (13), one sees that their forms would be identical if one were able to interpret $f_0 = \langle f \rangle$ and $\Delta f = \delta f$ *and* were able to identify the sink S with the divergence of the generalized flux $\boldsymbol{\Gamma} \doteq \langle \delta \boldsymbol{V} \delta f \rangle$. However, *this is not possible in general.* Frequently S vanishes (e.g., if one uses a Maxwellian distribution for f_0). However, $\partial_z \cdot \boldsymbol{\Gamma}$ does not always vanish. Suppose, for example, that in gyrokinetics the parallel nonlinearity $\delta E_\parallel \partial_{v_\parallel} \delta f$ is ignored. Then $\boldsymbol{\Gamma} \to \langle \delta \bar{\boldsymbol{V}}_E \delta f \rangle$, a turbulent $\boldsymbol{E} \times \boldsymbol{B}$ flux. The divergence $\boldsymbol{\nabla}_\perp \cdot \boldsymbol{\Gamma}$ would vanish if statistical homogeneity obtained in all directions. However, although that can be arranged for flux-tube simulations, it is not the case for global simulations with radially varying profiles. Indeed, it is that nonzero divergence that is responsible for the evolution of background profiles.

The implication of this observation is that the statistical mean of Δf does not vanish in general: $\langle \Delta f \rangle \neq 0$; that is, $\Delta f \neq \delta f$ [and, hence, $f_0 \neq \langle f \rangle$, which means that f_0 is not the steady-state background distribution]. This is unfortunate and must be remembered when attempting to interpret the simulation results analytically. Martin, Siggia, and Rose remarked in their fundamental paper on nonlinear statistical dynamics[58] that "Virtually no one does not take [the] first step" of writing the δf equation and the equation for the second cumulant $\langle \delta f \delta f \rangle$. But the Δf method takes a different first step.

B. The Δf-PIC algorithm

Various techniques have been proposed and explored for the solution of the GKE for Δf. The one of interest here is again called "particle-in-cell," although "gyrocenter-in-cell" would be more appropriate.

Many discussions of the Δf-PIC method preserve the full-f phraseology by referring to the particles as markers ("samplers" might be better). Note that for Δf the collection of markers no longer represents the dependent variable, even approximately. Instead, one adds the concept of a *marker weight* w that measures the value of Δf on a Lagrangian trajectory. That weight replaces the effective charge employed by Morse and Nielson. The proper treatment of marker weights lies at the core of the Δf-PIC algorithm.[59] But the basic estimate that the Δf Monte Carlo sampling noise scales with $\langle w^2\rangle$ should already be clear at this point.

Various interpretations of the weight function have been given in the literature, and certain confusions have arisen. For example, some authors have written

$$\Delta f(z,t) \propto \sum_i w_i(t)\,\delta(z-\tilde{z}_i(t)), \tag{14}$$

where i labels the markers. (The definition of, and equation for, the weight w will be discussed in Sec. III D 3.) However, the Δf of Eq. (10) *is a smooth field*, so the representation (14) cannot be literally correct. One is specifically not studying a many-body plasma, which is properly represented by a singular density (see Sec. III B below), but rather the GKE for a smooth distribution. If such an equation were solved exactly, no discreteness-related noise would emerge (although collective fluctuations would; see Sec. IV). It is important to distinguish the equation that is being solved from the various approximate methods of solution. (Of course, these remarks apply as well to full-f PIC.) To this end, consistent interpretations of the Δf-with-PIC algorithm were given by Aydemir[28] and Hu and Krommes;[5] for more discussion, see Sec. III D. Those insights are directly relevant to the analytical calculation of noise due to sampling error.

III. DISCRETENESS-INDUCED FLUCTUATIONS

Before we deal with the nuances of Monte Carlo sampling errors in continuum PDEs, it is useful to recall basic results on fluctuations due to particle discreteness.

The simplest case of the mean-square fluctuations of particle number in an ideal gas is discussed in several pedagogical ways by Landau and Lifshitz.[60] For any quantity A, define the fluctuation δA as $\delta A \doteq A-\langle A\rangle$, where the angle brackets denote the ensemble average. Let ΔN be the number of particles in a small volume element of size ΔV *(not the number of particles N in the entire system volume V).* Then

$$\left\langle\left(\frac{\delta(\Delta N)}{\Delta N}\right)^2\right\rangle = \frac{1}{\Delta N}. \tag{15}$$

This can be recovered by introducing the microdensity $\tilde{n}_s(\boldsymbol{x})=\Sigma_{i\in s}\delta(\boldsymbol{x}-\tilde{\boldsymbol{x}}_i)$, where the tildes denote random quantities and s denotes species. It is straightforward to multiply this by $\tilde{n}_{s'}(\boldsymbol{x}')$ and average with the assumptions of uniform background and statistical independence of distinct particles (here we assume an ideal gas) to find that the two-point density correlation function is[61]

$$C_{s,s'}(\boldsymbol{x},\boldsymbol{x}') \doteq \langle \delta n_s(\boldsymbol{x})\,\delta n_{s'}(\boldsymbol{x}')\rangle \tag{16a}$$

$$=\bar{n}_s\delta_{s,s'}[\delta(\boldsymbol{x}-\boldsymbol{x}')-V^{-1}]. \tag{16b}$$

Upon integrating over ΔV, one finds

$$\langle \delta(\Delta N)^2\rangle = \sum_{s,s'}\int_{\Delta V} d\boldsymbol{x}\int_{\Delta V} d\boldsymbol{x}'\,C_{s,s'}(\boldsymbol{x},\boldsymbol{x}') \tag{17a}$$

$$=\sum_{s,s'}\delta_{s,s'}\Delta N_s\left(1-\frac{\Delta V}{V}\right), \tag{17b}$$

which is approximately ΔN when $\Delta V \ll V$. However, if ΔV is taken to be the entire volume V, then one obtains $\langle\delta N^2\rangle=0$ identically; that must be true because the total number of particles in V has been assumed to be fixed. Note that this result does not require that either V or N approaches ∞.

A. Fluctuation-dissipation theorem for plasmas

In realistic systems with interparticle forces, the particles cannot be statistically independent. Although progress can be made in perturbation theory when the forces are weak [i.e., when the plasma discreteness parameter $\epsilon_p \doteq 1/\bar{n}\lambda_D^3 \ll 1$, where $\bar{n}\doteq N/V$ is the mean density, $\lambda_D \doteq k_D^{-1}$, and $k_D^2 \doteq \Sigma_s 4\pi(\bar{n}q^2)_s/T_s$], it is useful to be aware of the exact FDT, which holds (only) for systems in thermal equilibrium. A thorough treatment of the classical FDT has been given by Martin;[62] for discussion more specifically relevant to plasma physics, the book by Ecker[63] is quite readable. The FDT is obtained by considering the response to infinitesimal perturbations of the Gibbs N-body distribution $P_N(\Gamma) = Z^{-1}\exp[-H(\Gamma)/T]$, where H is the Hamiltonian, Γ is the collection of phase-space variables, and Z is the partition function. Under an external force $\boldsymbol{F}(\boldsymbol{x},t)$, let the resulting perturbation be written as $\Delta H(\Gamma)=-\int d\boldsymbol{x}\,\tilde{\boldsymbol{\alpha}}(\boldsymbol{x})\cdot\boldsymbol{F}(\boldsymbol{x},t)$, where the tilde denotes implicit dependence on Γ. This identifies the appropriate *state variable* $\boldsymbol{\alpha}$ conjugate to $\boldsymbol{F}$ [e.g., the negative of the microscopic charge density $\tilde{\rho}(\boldsymbol{x})=\Sigma_i q_i\delta(\boldsymbol{x}-\tilde{\boldsymbol{x}}_i)$ is conjugate to an external electrostatic potential ϕ]. The perturbing force induces a mean causal response $\Delta\langle\boldsymbol{\alpha}\rangle$, which at first order can be written in terms of a response tensor $\mathsf{K}(\boldsymbol{x},t;\boldsymbol{x}',t')$:

$$\Delta\langle\boldsymbol{\alpha}\rangle^{(1)}(\boldsymbol{x},t) = \int_{-\infty}^{t} dt'\int d\boldsymbol{x}'\,\mathsf{K}(\boldsymbol{x}-\boldsymbol{x}',t-t')\cdot\boldsymbol{F}(\boldsymbol{x}',t'). \tag{18}$$

The FDT relates the linear response matrix K to the two-point, equilibrium correlation tensor $\mathsf{C}_{\rm eq}(\boldsymbol{x},t,\boldsymbol{x}',t') \doteq \langle\delta\boldsymbol{\alpha}(\boldsymbol{x},t)\,\delta\boldsymbol{\alpha}(\boldsymbol{x}',t')\rangle_{\rm eq}$ as follows. With $\boldsymbol{r}\doteq\boldsymbol{x}-\boldsymbol{x}'$ and $\tau \doteq t-t'$, the theorem states that

$$\mathsf{K}(\boldsymbol{r},\tau) = -H(\tau)\frac{1}{T}\frac{\partial \mathsf{C}_{\mathrm{eq}}(\boldsymbol{r},\tau)}{\partial \tau}. \tag{19}$$

Thus, fundamentally, knowledge of equilibrium fluctuations determines the response of small perturbations away from equilibrium, which is reasonable. But Eq. (19) can sometimes be inverted by paying due attention to the symmetries and other properties of linear response matrices. For the case of scalar response (e.g., of induced charge to perturbing potential), one finds after Fourier transformation (see Appendix A for conventions) that

$$C_{\mathrm{eq}}(\boldsymbol{k},\omega) = 2T\omega^{-1}\,\mathrm{Im}\,K(\boldsymbol{k},\omega). \tag{20}$$

In this case, knowledge of linear response can be used to determine the equilibrium fluctuation spectrum. That may seem miraculous because no assumption has been made about the strength of the interparticle coupling; Eq. (20) is valid for strongly coupled plasmas, for example. But any perceived paradox can be resolved by noting that "linear" means "to first order in the perturbing force," not "to first order in the coupling"; terms of all orders in the interparticle potential are required to determine the forms of both K and C.

Let us deduce K for an electrostatic plasma. Now the dielectric function[64] $\mathcal{D}(\boldsymbol{k},\omega)$ is *defined* such that a small external potential $\Delta\phi^{\mathrm{ext}}$ creates in the plasma a *total* mean potential (including $\Delta\phi^{\mathrm{ext}}$) of value $\Delta\langle\phi\rangle^{\mathrm{tot}}(\boldsymbol{k},\omega) = \mathcal{D}^{-1}(\boldsymbol{k},\omega)\Delta\phi^{\mathrm{ext}}(\boldsymbol{k},\omega)$. To obtain the *induced* response (polarization) of the particles that is required by linear response theory, one must subtract $\Delta\phi^{\mathrm{ext}}$ to find $\Delta\langle\phi\rangle^{\mathrm{ind}} = (\mathcal{D}^{-1}-1)\Delta\phi^{\mathrm{ext}}$. Upon using Poisson's equation to replace $\Delta\langle\phi\rangle^{\mathrm{ind}}$ by $\Delta\langle\rho\rangle^{\mathrm{ind}}$, one identifies the charge-density response function as

$$K_{\rho\rho}(\boldsymbol{k},\omega) = -\frac{4\pi}{k^2}\left(\frac{1}{\mathcal{D}(\boldsymbol{k},\omega)} - 1\right). \tag{21}$$

Upon replacing the charge by the longitudinal electric field, one is led from Eq. (20) to the familiar result

$$\frac{C_{EE}(\boldsymbol{k},\omega)}{8\pi} = -\frac{T}{\omega}\,\mathrm{Im}\left(\frac{1}{\mathcal{D}(\boldsymbol{k},\omega)}\right) = \frac{T}{\omega}\frac{\mathrm{Im}\,\mathcal{D}(\boldsymbol{k},\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2}. \tag{22}$$

Note that this result has the standard shielding form (2).

It must be stressed that this exact formula is not necessarily helpful, because (like all response functions K) $\mathcal{D}^{-1}$ contains terms of all orders in the fluctuations; Eq. (22) is in general a very difficult transcendental equation for C. However, for weak coupling with $T = O(\epsilon_p)$ [and for $k\lambda_D = O(1)$ and $\omega/\omega_p = O(1)$], it is sufficient to use the lowest-order dielectric $\mathcal{D}^{(0)}$, whose determination is a standard exercise in linearized Vlasov theory. Alternatively, it is possible to integrate Eq. (22) over all frequencies exactly by first noting that a response function for stable plasma must be analytic in the upper half of the ω plane, then using the Kramers-Kronig relations (or the methodology that leads to them). Thus, integrate the first form of Eq. (22) over all real frequencies,

$$\frac{C_{EE}(\boldsymbol{k})}{8\pi} = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{C_{EE}(\boldsymbol{k},\omega)}{8\pi} \tag{23a}$$

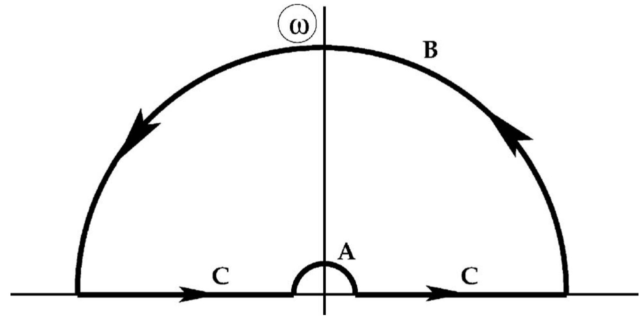

FIG. 2. The contour integration used to calculate the equilibrium wavenumber spectrum. The arc B is at ∞.

$$= -T\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{1}{\omega}\,\mathrm{Im}\left(\frac{1}{\mathcal{D}(\boldsymbol{k},\omega)}\right). \tag{23b}$$

If this result is to be well defined, it must be the case that the apparent singularity at $\omega=0$ is canceled by a zero of $\mathrm{Im}(\mathcal{D}^{-1})$. Thus one may proceed as follows (see Fig. 2). First, deform the ω contour to traverse a vanishingly small semicircle around the origin; the contribution from that contour is negligible because the integrand is smooth in the vicinity of $\omega=0$. Next, bring Im to the outside of the integral; although one now has a singularity at $\omega=0$, the contour no longer intersects it. Finally, close the contour at ∞ and use Cauchy's theorem to deduce that $\int_C = -\int_A - \int_B$. One obtains

$$\frac{C_{EE}(\boldsymbol{k})}{8\pi} = \frac{1}{2}T\left(\frac{1}{\mathcal{D}(\boldsymbol{k},\infty)} - \frac{1}{\mathcal{D}(\boldsymbol{k},0)}\right). \tag{24}$$

Upon using the static shielding result[65]

$$\mathcal{D}(\boldsymbol{k},0) = 1 + k_D^2/k^2 \tag{25}$$

and the vacuum limit $\mathcal{D}(\boldsymbol{k},\infty)=1$, one is led to

$$\frac{C_{EE}(\boldsymbol{k})}{8\pi} = \frac{T/2}{1+k^2\lambda_D^2}. \tag{26a}$$

Equation (26a) uses the continuous spatial Fourier transform. In a finite-sized periodic box, a Fourier series representation is usually advantageous. With the conventions in Appendix A, one has $C_{EE}(\boldsymbol{k}) = VC_{EE,\boldsymbol{k}}$, so a dimensionless representation of the result (26a) is

$$\frac{C_{EE,\boldsymbol{k}}}{8\pi\bar{n}T} = \frac{1}{N}\frac{1/2}{1+k^2\lambda_D^2}. \tag{26b}$$

There are important lessons to be learned from Eqs. (26a) and (26b):

(1) At short wavelengths, the 1 in the denominator may be neglected and Eqs. (26a) and (26b) reduce to the result for statistically independent particles, which can be obtained by proceeding from the Fourier transform of Eq. (16b).

(2) At long wavelengths, dielectric shielding is important. That effect is intrinsically a nonlinear phenomenon (it depends on corrections to the free-streaming motion of the particles). Exact nonlinear results in many-body theory are rare. Thus, comparison of formula (26b) with

numerical results affords an important test of the nonlinear parts of a simulation code, and that has been done.[66]

(3) The presence of $\frac{1}{2}T$ in Eqs. (26a) and (26b) suggests a tendency toward statistical equilibration. At long wavelengths, this can be quantified by considering the energy in the normal modes. For classical equilibrium plasmas in the electrostatic approximation, the normal modes are the Langmuir oscillations $\omega \approx \pm\omega_p$.[67] If one integrates Eq. (22) over a resonance [(real) ω near a complex zero $\Omega + i\gamma$ of $\mathcal{D}(\omega)$ that lies slightly below the real axis, with $|\gamma/\Omega| \ll 1$] with the aid of the formula

$$\frac{1}{|\mathcal{D}(\boldsymbol{k},\omega)|^2} \approx \frac{1}{|\partial\mathcal{D}(\boldsymbol{k},\omega)/\partial\omega|^2_{\Omega_{\boldsymbol{k}}}} \frac{1}{|\gamma_{\boldsymbol{k}}|}\pi\delta(\omega - \Omega_{\boldsymbol{k}}), \tag{27}$$

one can prove that (a) the Langmuir oscillations carry all of the fluctuation energy, and (b) each normal mode carries $\frac{1}{2}T$ of energy (including both electrostatic field energy as well as mechanical sloshing).

(4) For $k\lambda_D \gg 1$, erstwhile Langmuir oscillations are heavily (exponentially) Landau damped, so do not qualify as normal modes. Although C_{EE} is reduced below $\frac{1}{2}T$, it is not exponentially small. Hence one concludes that for $k\lambda_D \gg 1$ fluctuation energy is not carried by normal modes; it resides merely in the unshielded fields of the essentially independent test particles.

(5) Formula (26b) contains the factor N^{-1}, N being the total number of particles in the box. This may appear to differ from (15), which contains the number of particles ΔN in a volume element much smaller than the system size. But if one sums over all modes within a Debye sphere (inserting a k-dependent function a to allow for the possibility of various $\boldsymbol{k}$ weightings, where $a \equiv 1$ for C_{EE}), one finds that[68] $N^{-1}\Sigma_{|\boldsymbol{k}|<k_D} a(k\lambda_D)/(1+k^2\lambda_D^2) = O(1/\bar{n}\lambda_D^3)$, i.e., the effective $\Delta N \sim \bar{n}\lambda_D^3$ is of the order of the number of particles within the Debye *shielding volume*. The presence of such a shielding volume (a measure of the total strength of the fluctuations) seems to be not universally appreciated, but it is inevitable whenever sums over Fourier intensities are performed. Obviously a similar shielding volume must arise in calculations of gyrokinetic noise.[1]

B. Introduction to the Klimontovich formalism

So far I have discussed the consequences of the rigorous FDT, which is valid only in thermal equilibrium. However, fluctuations in stable plasmas that are slightly nonequilibrium are also of interest. The Klimontovich formalism[14] is an elegant and technically convenient way to proceed, particularly for weakly coupled plasmas. I introduce the formalism here, as it will be required in several places later in the article.

The Klimontovich phase-space microdensity is

$$\tilde{N}_s(z,t) \doteq \frac{1}{\bar{n}_s}\sum_{i\in s}\delta(z - \tilde{z}_i(t)). \tag{28}$$

Here z is the collection of observer variables labeling a single generic particle of species s, and $\tilde{z}_i(t)$ is the trajectory of the ith particle (it is random because it evolves from a randomly distributed initial condition). The ensemble average of $\tilde{N}$ is the one-particle "distribution function" $f(z,t) = \langle\tilde{N}(z,t)\rangle$, normalized such that $V^{-1}\int d\boldsymbol{x}d\boldsymbol{v}\, f(\boldsymbol{x},\boldsymbol{v},t) = 1$; that is, $f(z,t) = VP_1(z,t)$, where P_1 is the one-particle probability density function (PDF). A consequence of this normalization is that density is obtained as $n_s(\boldsymbol{x},t) = \bar{n}_s\int d\boldsymbol{v}\, f_s(\boldsymbol{x},\boldsymbol{v},t)$.

Time differentiation of Eq. (28) leads to the Klimontovich equation $\partial_t\tilde{N} + \partial_z\cdot(\tilde{\dot{z}}\tilde{N}) = 0$. This form of the equation is valid even for dissipative dynamics; however, when phase-space volume elements are conserved, i.e., $\partial_z\cdot\tilde{\dot{z}} = 0$, one obtains the possibly more familiar form

$$\partial_t\tilde{N} + \tilde{\dot{z}}\cdot\partial_z\tilde{N} = 0. \tag{29}$$

Equation (29) should not be confused with the Liouville equation for the N-body PDF $P_N(\Gamma)$. Γ is $6N$-dimensional, whereas z is 6-dimensional. More importantly, the Liouville equation is a linear PDE, while Eq. (29) is in general nonlinear because $\tilde{\dot{z}}$ in general depends on $\tilde{N}$. For example, the Klimontovich equation for an unmagnetized, electrostatic plasma is

$$\partial_t\tilde{N}(\boldsymbol{x},\boldsymbol{v},t) + \boldsymbol{v}\cdot\nabla\tilde{N} + (q/m)\tilde{\boldsymbol{E}}(\boldsymbol{x},t)\cdot\partial_{\boldsymbol{v}}\tilde{N} = 0, \tag{30}$$

where $\tilde{\boldsymbol{E}}$ is obtained from the microscopic charge density $\tilde{\rho} = \Sigma_s(\bar{n}q)_s\int d\boldsymbol{v}\,\tilde{N}_s(\boldsymbol{x},\boldsymbol{v},t)$ via Poisson's equation. Thus the Klimontovich equation for plasmas is quadratically nonlinear,[69] possessing a form generically similar to other quadratically nonlinear equations such as the Navier-Stokes equation. It suffers from all of the difficulties of those continuum equations (and more because of the singular initial conditions on $\tilde{N}$). However, progress can be made in the limit of weak coupling, $\epsilon_p \ll 1$.

Consider the calculation of the two-point charge-charge correlation function $\langle\delta\rho(\boldsymbol{x},t)\delta\rho(\boldsymbol{x}',t')\rangle$ (or its Fourier transform, the fluctuation spectrum). $\delta\rho$ follows from δN. The rigorous equation for δN is (for $\langle\boldsymbol{E}\rangle = \boldsymbol{0}$)

$$\partial_t\delta N + \boldsymbol{v}\cdot\nabla\delta N + (q/m)\delta\boldsymbol{E}\cdot\boldsymbol{\partial}_{\boldsymbol{v}} f = -(q/m)\partial_{\boldsymbol{v}}\cdot(\delta\boldsymbol{E}\,\delta N - \langle\delta\boldsymbol{E}\,\delta N\rangle), \tag{31}$$

where $f(\boldsymbol{x},\boldsymbol{v},t) \doteq \langle\tilde{N}(\boldsymbol{x},\boldsymbol{v},t)\rangle$ is the one-particle distribution function. When the right-hand side of Eq. (31) is neglected (appropriate for nearly equilibrium, stable, and weakly coupled plasmas), one is left with

$$(R^{(0)})^{-1}\delta N = 0, \tag{32}$$

where $R^{(0)}$ is Green's function for the linearized Vlasov equation. That $R^{(0)}$ emerges is the starting point for proofs of Rostoker's Superposition Principle[70,71] and derivations of the usual test-particle methods for evaluating weakly coupled fluctuation spectra.[46] Thus it is straightforward to find that in the electrostatic limit

$$\langle \delta \boldsymbol{E}\, \delta \boldsymbol{E}\rangle(\boldsymbol{k},\omega) = \frac{2\pi \boldsymbol{\epsilon}_{\boldsymbol{k}} \boldsymbol{\epsilon}_{\boldsymbol{k}}^*}{|\mathcal{D}^{(0)}(\boldsymbol{k},\omega)|^2} \sum_s (\bar{n}q^2)_s \int d\boldsymbol{v}\, \delta(\omega - \boldsymbol{k}\cdot\boldsymbol{v}) f_s(\boldsymbol{v}), \tag{33}$$

where $\boldsymbol{\epsilon}_{\boldsymbol{k}} \doteq -4\pi i \boldsymbol{k}/k^2$ is the Fourier-space representation of the field of a unit point charge.

Let us compare the nonequilibrium result (33) to the equilibrium prediction (22) of the FDT. Since the electrostatic dielectric is (to lowest order in ϵ_p)

$$\mathcal{D}^{(0)}(\boldsymbol{k},\omega) = 1 + \sum_s \frac{\omega_{ps}^2}{k^2} \int d\boldsymbol{v} \frac{\boldsymbol{k}\cdot \partial f_s/\partial \boldsymbol{v}}{\omega - \boldsymbol{k}\cdot\boldsymbol{v} + i\epsilon} \tag{34}$$

(ϵ being a positive infinitesimal), one has

$$\operatorname{Im} \mathcal{D}^{(0)} = -\pi \sum_s \frac{\omega_{ps}^2}{k^2} \int d\boldsymbol{v}\, \delta(\omega - \boldsymbol{k}\cdot\boldsymbol{v}) \boldsymbol{k}\cdot \frac{\partial f_s}{\partial \boldsymbol{v}}. \tag{35}$$

The key difference is thus that the equilibrium formula involves $\int d\boldsymbol{v}\, \delta(\omega - \boldsymbol{k}\cdot\boldsymbol{v}) \boldsymbol{k}\cdot \partial_{\boldsymbol{v}} f$ (reflecting the fact that the dissipation mechanism in the FDT involves the Landau wave-particle resonance), whereas the more general nonequilibrium result involves $\int d\boldsymbol{v}\, \delta(\omega - \boldsymbol{k}\cdot\boldsymbol{v}) f$ (reflecting the fact that the fluctuations are "Cerenkov"-emitted by the moving test particles). In thermal equilibrium those two processes are in balance. Upon evaluating $\mathcal{D}^{(0)}$ with a Maxwellian distribution function f_M, one finds

$$\frac{C_{EE}(\boldsymbol{k},\omega)}{8\pi} = \begin{cases} \pi T \sum_s \left(\frac{k_{Ds}^2}{k^2}\right) \int d\boldsymbol{v}\, \delta(\omega - \boldsymbol{k}\cdot\boldsymbol{v}) f_{M,s}(\boldsymbol{v}) \\ \qquad \text{(equilibrium)} \\ \pi \sum_s T_s \left(\frac{k_{Ds}^2}{k^2}\right) \int d\boldsymbol{v}\, \delta(\omega - \boldsymbol{k}\cdot\boldsymbol{v}) f_s(\boldsymbol{v}) \\ \qquad \text{(nonequilibrium)}. \end{cases} \tag{36}$$

Thus the nonequilibrium Klimontovich calculation reduces correctly and simply to the prediction of the FDT. This emphasizes that the FDT, although important and profound, is not required for practical calculations of discreteness effects in stable plasmas if the assumption of weak coupling is appropriate. When some researchers speak of the inapplicability of the FDT for nonequilibrium calculations, they are referring not to the trivial differences between the equilibrium and near-equilibrium formulas (36) but rather to the possibility that the result for $C(\boldsymbol{k},\omega)$ may be strongly modified when the plasma is unstable and turbulent.

C. Fluctuation-dissipation theorem for gyrokinetics

Let us consider extensions of these results to gyrokinetics. (In this article, I refer only to *low-frequency* gyrokinetics: $\omega \ll \omega_{ci}$.) Modern GK theory has been recently reviewed by Brizard and Hahm;[72] some introductory remarks can be found in Refs. 7 (Appendix C) and 73. Here I do not require all of the (important) technology of differential one-forms, Lie transforms, etc. However, I do need to emphasize that *gyrokinetic plasmas are distinct dynamical systems in their own right,* with their own dielectric and fluctuation properties. Specifically, a GK plasma consists of a collection of gyrocenters moving with nonlinear $\boldsymbol{E}\times\boldsymbol{B}$ advection in a *gyrokinetic vacuum*[4,22] possessing a nontrivial permittivity that captures the effect of the ion polarization drift. The properties of the GK vacuum dictate that applications of fluctuation-dissipation theory must be made with care.

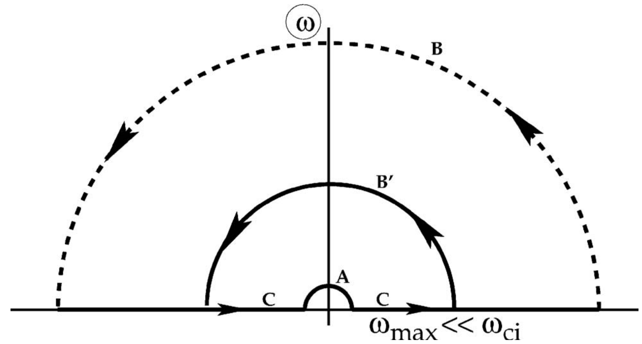

FIG. 3. Gyrokinetic contour integration. The contour is closed along an arc B' with $|\omega| \ll \omega_{ci}$. The dashed arc B is at true ∞.

1. The gyrokinetic vacuum and gyrokinetic Poisson equation

Consider a GK plasma in thermal equilibrium. The shielding effects of ion polarization drift lead one to correctly conclude on physical grounds that fluctuations in such plasmas should be small relative to the classical prediction (26a) and (26b). But note that this result does not follow from Eqs. (26a) and (26b) by taking, say, the limit of large magnetic field $\boldsymbol{B}$. Equation (24) is correct for arbitrarily magnetized (electrostatic) plasmas. So is Eq. (25), which is independent of $\boldsymbol{B}$. (That can be understood by noting that $\boldsymbol{B}$ does not appear in the Hamiltonian; all one-time properties of a Gibbsian plasma are $\boldsymbol{B}$-independent.) Thus an arbitrarily magnetized plasma in thermal equilibrium has the wave-number spectrum (26a) and (26b), the size of which is not reduced in any way by magnetic-field effects.

Although static properties of a magnetized plasma are unaffected by the presence of a magnetic field, however large, the time required to approach a Gibbsian state definitely does depend on $\boldsymbol{B}$. Thus so does $\mathcal{D}(\boldsymbol{k},\omega)$; this is well known by students of plasma waves,[74] who must wade through a morass of Bessel functions. If one is careful, one can exploit this fact to obtain the correct GK equilibrium wave-number spectrum. The calculation to be described now was first performed by Krommes *et al.*[22] It is somewhat clumsy and has been superseded by calculations based directly on the GKE, to be reviewed shortly. But it is instructive to extract the result from the full plasma response. Thus, let us integrate only over frequencies such that $\omega \ll \omega_{ci}$. One may follow the same procedure as diagrammed in Fig. 2; however, now the closed contour B' at "∞" (see Fig. 3) still obeys $|\omega| \ll \omega_{ci}$. Thus all gyration harmonics except $n=0$ are asymptotically small and can be dropped; call the resulting approximation $\mathcal{D}_<(\boldsymbol{k},\omega)$. Because along B' $|\omega|$ is supposedly large compared to any modes of interest, one may evaluate $\mathcal{D}_<$ at $\omega=\infty$, thereby obtaining[22] for a Maxwellian distribution in $\boldsymbol{v}_\perp$

$$\mathcal{D}_<(\boldsymbol{k},\infty) \equiv \epsilon_{\rm GV}(\boldsymbol{k}) \doteq 1 + \sum_s \left(\frac{k_{Ds}^2}{k^2}\right)(1-\Gamma_s) \quad (37a)$$

$$\approx 1 + \left(\frac{k_{Di}^2}{k^2}\right)(1-\Gamma), \quad (37b)$$

where $\Gamma_s(\boldsymbol{k}) \doteq \int d\boldsymbol{v}_\perp J_0^2(k_\perp v_\perp/\omega_{cs}) f_{M,s}(v_\perp) = I_0(b_s)e^{-b_s}$ [$b_s \doteq k_\perp^2\rho_s^2$, $\rho_s \doteq v_{ts}/\omega_{cs}$, $v_{ts} \doteq (T/m)_s^{1/2}$] and $\Gamma \equiv \Gamma_i$. (For electrons, the gyroradius ρ_e is so small that it is adequate to approximate $\Gamma_e \approx 1$.) One may identify $\epsilon_{\rm GV}$ with the effective *dielectric permittivity of the gyrokinetic vacuum.*

The GK equilibrium wave-number spectrum now follows immediately from formula (24). Before discussing its consequences, however, let us consider the modern version of this calculation. As reviewed in Ref. 72 (see also Appendix C of Ref. 7 and pedagogical introductory remarks in Ref. 73), the GK-Poisson system[75] is derived by systematic Hamiltonian transformation of the particle variables to those of the gyrocenter, the latter being defined such that μ is conserved. The polarization effect then appears in the Poisson equation (naturally stated in particle variables) when the charge is evaluated in terms of the gyrocenter PDF. For uniform $\boldsymbol{B}$ (appropriate for thermal equilibrium), the result is[76]

$$\frac{\partial F}{\partial t} + v_\parallel \nabla_\parallel F + \bar{\boldsymbol{V}}_E \cdot \boldsymbol{\nabla} F + \left(\frac{q}{m}\right)\bar{E}_\parallel \frac{\partial F}{\partial v_\parallel} = 0, \quad (38a)$$

$$-(\nabla^2 + \hat{\epsilon}_\perp \nabla_\perp^2)\phi = 4\pi\rho_G. \quad (38b)$$

Here the overline indicates an effective quantity felt by the gyrocenter. In $\boldsymbol{k}$ space, this introduces the Bessel function $J_0(k_\perp v_\perp/\omega_c)$ as a multiplier, e.g., $\bar{E}_\parallel \doteq J_0 E_\parallel$. The polarization effect is represented by $\hat{\epsilon}_\perp$, a spatial operator whose $\boldsymbol{k}$-space representation is

$$\epsilon_\perp(\boldsymbol{k}) \doteq \left(\frac{k_{Di}^2}{k_\perp^2}\right)[1-\Gamma(\boldsymbol{k})] = \left(\frac{k^2}{k_\perp^2}\right)[\epsilon_{\rm GV}(\boldsymbol{k}) - 1]. \quad (39)$$

The spatial Fourier transform of Eq. (38b) thus introduces the same $\epsilon_{\rm GV}$ that arose in Eq. (37b), and the GK Poisson equation can be written variously as

$$-\hat{\epsilon}_{\rm GV}\nabla^2\phi = 4\pi\rho_G \quad \text{or} \quad \epsilon_{\rm GV}(\boldsymbol{k})k^2\phi_{\boldsymbol{k}} = 4\pi\rho_{\boldsymbol{k}}^G. \quad (40)$$

Ion polarization drift is a fluid effect; it survives in the cold-ion limit $T_i \to 0$.[77] In that limit,

$$\epsilon_\perp(\boldsymbol{k}) \approx k_{Di}^2\rho_i^2 = \rho_s^2/\lambda_{De}^2 = \omega_{pi}^2/\omega_{ci}^2, \quad (41)$$

where[78] $\rho_s \doteq c_s/\omega_{ci}$ and $c_s \doteq (ZT_e/m_i)^{1/2}$ (Z is the atomic number). For realistic fusion parameters, typically[79] $\omega_{pi}^2/\omega_{ci}^2 \gg 1$; this defines the *gyrokinetic regime.*[22] For the usual case $k_\parallel^2 \ll k_\perp^2$, this implies that ion polarization charge dominates the original $\nabla^2\phi$ of Poisson. The approximate GK Poisson equation $-\hat{\epsilon}_\perp \nabla_\perp^2 \phi = 4\pi\rho_G$ is a statement of quasineutrality in the laboratory (particle) coordinate system, expressed however in terms of the gyrocenter charge density. (Note that the limit $T_i \to 0$ with T_e=const is not permitted for thermal equilibrium, which requires $T_i = T_e$.)

2. The gyrokinetic fluctuation-dissipation theorem

One may apply the FDT to the new GK dynamical system. The GK charge-density response function is the generalization of Eq. (21),

$$K_{\rho\rho}^G(\boldsymbol{k},\omega) = -\frac{1}{\epsilon_{\rm GV}(\boldsymbol{k})}\left(\frac{4\pi}{k^2}\right)\left(\frac{1}{\mathcal{D}_G(\boldsymbol{k},\omega)} - 1\right); \quad (42)$$

note the presence of $\epsilon_{\rm GV}$ in the denominator. If the perpendicular velocity-space distribution is taken to be Maxwellian (with no spatial gradients), the linear GK dielectric is readily found to be

$$\mathcal{D}_G^{(0)}(\boldsymbol{k},\omega) = 1 + \sum_s \frac{\omega_{ps}^2\Gamma_s}{\epsilon_{\rm GV}k^2}\int dv_\parallel \frac{k_\parallel \partial_{v_\parallel} F_s}{\omega - k_\parallel v_\parallel + i\epsilon} \quad (43)$$

(see Appendix B for more discussion). This function (not to be confused with $\mathcal{D}_<$) has the clean limits $\mathcal{D}_G^{(0)}(\boldsymbol{k},\infty) = 1$ and, in thermal equilibrium,

$$\mathcal{D}_G^{(0)}(\boldsymbol{k},0) = \frac{1}{\epsilon_{\rm GV}(\boldsymbol{k})}\left(1 + \frac{k_D^2}{k^2}\right), \quad (44)$$

where Eq. (37a) was used. Upon integrating Eq. (42) over all frequencies and using these limits, one obtains the equilibrium $\boldsymbol{k}$ spectrum for a GK many-body plasma,

$$\frac{C_{EE}^G(\boldsymbol{k})}{8\pi} = \frac{T/2}{\epsilon_{\rm GV}(\boldsymbol{k})}\left(1 - \frac{\epsilon_{\rm GV}}{1 + k_D^2/k^2}\right) \quad (45a)$$

$$= \frac{T/2}{\epsilon_{\rm GV}(\boldsymbol{k})}\left(\frac{(k_{De}^2 + k_{Di}^2\Gamma)/k_D^2}{1 + k^2\lambda_D^2}\right). \quad (45b)$$

The numerator of the last parenthesized fraction is of order unity,[80] so we have recovered a result quite similar to Eq. (26a) except for the presence of the large GK permittivity in the denominator. One concludes that *thermal fluctuations in a gyrokinetic plasma are much smaller than those in a conventional many-body plasma.*

Formula (45b) can be integrated over all $\boldsymbol{k}$. Dimensionally it is easy to see that the GK shielding volume is $O(\lambda_{\rm De}\rho_s^2)$. To make this precise, one must incorporate cutoff factors relating to finite-size particles, as done in Ref. 1. The details depend on the specific simulation algorithm[81] and are thus beyond the scope of this article. But the existence of such a shielding volume is clear.

3. Gyrokinetic fluctuations and normal modes

We have arrived at the spectrum (45b) by assuming only weak coupling (which justifies use of the lowest-order dielectric); no reference to normal modes was made. However, a basic understanding of those modes is often useful, particularly when considering the transition from stable to unstable plasmas. The GK normal modes in the absence of magnetic drifts are discussed in Appendix C. One finds two branches: high-frequency modes $\omega = \pm\Omega_H$ that in the electrostatic limit are the GK version of Langmuir oscillations, and the ion sound waves (which are heavily Landau damped in thermal equilibrium). In thermal equilibrium and for $k_\perp\rho_s \ll 1$, the Ω_H modes are weakly damped and can be shown to carry the bulk of the fluctuation energy, just as do the Langmuir waves in the unmagnetized plasma. It is well known that the sound wave is the nucleus of the conventional electron drift wave, which arises in the presence of a background density gradient. I shall consider the consequences of the drift wave later in the context of steady-state but nonequilibrium spectra.

4. Gyrokinetic fluctuations with an adiabatic species

In simulations of ion- or electron-temperature-gradient-driven (ITG or ETG) modes, it is popular to assume that one species is adiabatic ($\delta n_s/\bar{n}_s = -q_s\delta\phi/T_s$) from the outset; then only one species needs to be simulated. This useful approximation eliminates the discreteness of the adiabatic species, so one expects that the thermal level of fluctuations should be reduced. To calculate that level for weakly coupled plasmas, it is simplest to apply the Klimontovich formalism, whose predictions are valid even for slightly nonequilibrium situations. Such a calculation was done by Hammett[1,82] for ETG simulations (adiabatic ions); it provides an interesting exercise for the serious student of gyrokinetics. Here, I quote the result for adiabatic electrons:[83] $\langle\delta E^2\rangle(\boldsymbol{k},\omega) \propto \operatorname{Im}\chi_i/|1+\chi_i+\chi_{e0}|^2$, where $\chi_{e0} = (\epsilon_{GV}k^2\lambda_{\mathrm{De}}^2)^{-1}$ is the static electron susceptibility. This can be integrated exactly over the frequency.[84] In place of Eq. (45b), one finds

$$\frac{C_{EE}^{Ge}(\boldsymbol{k})}{8\pi} = \frac{T_i/2}{\epsilon_{\mathrm{GV}}(\boldsymbol{k})}\frac{k_{Di}^2\Gamma/k_D^2}{(1+k_{\mathrm{De}}^2/\epsilon_{\mathrm{GV}}k^2)(1+k^2\lambda_D^2)}, \tag{46}$$

which can be seen to be smaller than formula (45b) (the numerator is smaller and the denominator is larger). Such details are important when one attempts to establish quantitative connections with the simulations.[1]

D. Sampling noise in the Δf algorithm

If we were actually dealing with GK many-particle plasmas, the next logical step would be to describe the extension of the results of the last section to unstable, turbulent regimes. I shall describe such results in Sec. IV. However, the widespread use of the Δf algorithm requires us to first consider further issues relating to the very meaning of noise in such simulations. Indeed, that algorithm is a procedure for solving a kinetic equation in which the fluctuations stemming from particle discreteness do not appear explicitly, their effect having been replaced by an integro-differential collision operator. In the strictly collisionless limit, the kinetic equation reduces to the GK Vlasov equation. That equation contains no effects due to particle discreteness at all!

The GKE is a PDE that evolves in five-dimensional (5D) phase space. Various numerical techniques are available for its solution. For example, conventional Fourier transformation and/or finite-difference techniques can be applied. Generically this is known as the "continuum" or "Vlasov" approach, examples of which are the codes GS2,[85] GENE,[86] and GYRO.[87]

1. Monte Carlo sampling

Monte Carlo sampling provides an alternate solution procedure, and it is on this that I shall focus. The method can be motivated by recognizing that in order to evolve Δf one requires the electric field $\Delta\boldsymbol{E}$, which is a particular phase-space moment of Δf. Generally, one can represent such moments as

$$M_s(z,t) \doteq \sum_{\bar{s}} \int d\bar{z}\, M_{s,\bar{s}}(z,\bar{z})\Delta f_{\bar{s}}(\bar{z},t). \tag{47}$$

For example, one obtains $\Delta\boldsymbol{E}$ if the kernel $M_{s,\bar{s}}(z,\bar{z})$ is taken to be the Green's function associated with Poisson's equation. Because the $\bar{z}$ integral is over a space of moderately high dimension (five), Monte Carlo sampling is suggested as an expeditious approach to evaluating that integral.

In fact, such a 5D integral is not actually done in the PIC approach. That method deals with a nongridded 2D velocity space but deposits particles onto a 3D spatial grid in order to calculate the collective charge density. I shall return to this important issue,[88] but it is useful to first review the approximation of integrals by basic Monte Carlo sampling.[89] (A more complete version of the discussion in this paragraph can be found in Ref. 28.) Consider the integral $I = \int_0^L d\bar{x}\, f(\bar{x})$, where $f(x)$ is specified. This can be written in the form

$$I = L\int_0^L d\bar{x}\, P(\bar{x})f(\bar{x}) = L\langle f\rangle, \tag{48}$$

where $P(x) \doteq L^{-1}$ is the PDF of a random variable $\tilde{x}$ that is distributed uniformly over the interval $(0,L)$. It is well known that an unbiased estimator of $\langle f\rangle$ is $\langle f\rangle \approx \tilde{f} \doteq N^{-1}\sum_{i=1}^N f(\tilde{x}_i)$, where the $\tilde{x}_i$ are samples from the uniform distribution. Also, one can show that the variance $\langle(\tilde{I}-I)^2\rangle$ is proportional to N^{-1}, so accuracy can be improved by taking more samples, although convergence is slow. This method is distinctly inefficient in one dimension; however, it may provide the only practical way of evaluating integrals in spaces of sufficiently high dimensionality. Note that one can write $\tilde{I} \doteq L\tilde{f}$ as

$$\tilde{I} = \frac{L}{N}\sum_i \int_0^L d\bar{x}\,\delta(\bar{x}-x_i)f(\bar{x}) = \int_0^L d\bar{x}\,\tilde{N}(\bar{x})f(\bar{x}), \tag{49}$$

where the Klimontovich microdensity $\tilde{N}(x) \doteq \bar{n}^{-1}\sum_{i=1}^N \delta(x-\tilde{x}_i)$ has appeared. (Here $\bar{n} \doteq N/L$ is the mean density of sampling points.) Thus, except for normalization, the Monte Carlo procedure amounts to the replacement in Eq. (48) of the smooth PDF $P(x)$ by its singular counterpart $\tilde{N}(x)$.

2. Markers and weights

I now return to the Δf problem. To evaluate formula (47) by exact analogy, one should write it in the form of a phase-space average. In principle, one may average over (sample from) any distribution function $F_m(z,t)$; by multiplying and dividing by F_m, one finds that Eq. (47) can be written as

$$M_s(z,t) = \sum_{\bar{s}} V\int \frac{d\bar{z}}{V}F_{m,\bar{s}}(\bar{z},t)M_{s,\bar{s}}(z,\bar{z})\left(\frac{\Delta f_{\bar{s}}(\bar{z},t)}{F_{m,\bar{s}}(\bar{z},t)}\right) \tag{50a}$$

$$=V\sum_{\bar{s}}\langle M_{s,\bar{s}}(z,\bar{z})w_{\bar{s}}(\bar{z},t)\rangle_{F_m}, \tag{50b}$$

where the *weight function* has been defined to be

$$w \doteq \Delta f/F_m. \tag{51}$$

Thus moments have been expressed in terms of an "ensemble" average taken over F_m. However, this formulation is useful only if one can find a computationally tractable equation for the time-dependent weight. That can be accomplished by choosing F_m to be the *marker distribution*, namely $F_m \doteq \langle \widetilde{N}_m\rangle$, where the marker trajectories that define the Klimontovich marker microdensity $\widetilde{N}_m$ obey the characteristic equations of motion. Then, when M_s is evaluated by Monte Carlo sampling, it is seen that w is required only at the phase-space position of the markers, since one has

$$\widetilde{M}_s(z,t) \approx \sum_{\bar{s}}\int d\bar{z}\,\widetilde{N}_{m,\bar{s}}(\bar{z},t)M_{s,\bar{s}}(z,\bar{z})\widetilde{w}_{\bar{s}}(\bar{z},t). \tag{52}$$

(I have written a tilde on $\widetilde{w}$ because w evaluated along the marker trajectories will be random in the same sense as $\widetilde{N}_m$ is; see the end of the next section for more discussion.) I shall demonstrate shortly that a relatively simple equation can be written for $\widetilde{w}$. Thus we see that the sampling procedure amounts to a generalized "particle" (really marker) simulation in which both the phase-space position and weight are evolved for each particle and the fields are calculated self-consistently at each time step.

This argument shows how the Monte Carlo viewpoint leads naturally to the introduction of the particular dimensionless weight function defined by Eq. (51). However, it does not adequately capture the PIC methodology, in which particles are deposited onto a spatial grid and specialized techniques (e.g., fast Fourier transforms) are then used to calculate the field. Thus, the spatial part of the integral is not performed by Monte Carlo sampling. Furthermore, the dimensions of the grid cells are constrained by physics considerations that must hold no matter what numerical algorithm is employed. Thus, it would seem that arguments about the relative efficacy of the PIC approach from the point of view of Monte Carlo integration should be based on a 2D velocity space[88] rather than a 5D phase space. 2D is too small to make PIC the clear winner, although detailed analyses of the operation counts for various algorithms and architectures are well beyond the scope of this article. Nevertheless, PIC is an intuitive method that is widely used, so I shall proceed with its analysis in the context of Δf.

3. The weight equation

I shall now derive the rigorous evolution equation for $w(z,t)$ (a smooth field). From the definition (51),

$$\frac{\partial w}{\partial t}=\frac{1}{F_m}\frac{\partial \Delta f}{\partial t}-\frac{w}{F_m}\frac{\partial F_m}{\partial t}. \tag{53}$$

For $\partial_t\Delta f$, one may use Eq. (10). (I shall ignore the $\boldsymbol{V}_0$ term; if it is nonzero, its effect can be incorporated into a modified $\hat{L}$ if $\partial_z\cdot\boldsymbol{V}_0=0$.) To find an evolution equation for the smooth marker distribution F_m, one may begin with the microscopic Klimontovich-type equation

$$(\partial_t-\hat{L})\widetilde{N}_m+\partial_z\cdot(\Delta\boldsymbol{V}\widetilde{N}_m)=0. \tag{54}$$

Here I have used the fundamental definition (28) and the prescription that the markers evolve under the action of the fields arising from Δf: $\Delta\boldsymbol{V}\doteq\boldsymbol{V}[\Delta f]$. Note specifically that these dynamics do not include the microscopic fields that would arise from individual discrete particles. One can find an equation for F_m by averaging Eq. (54), but one must be very careful. One may not perform a statistical average over all turbulent scales of motion, as in the theory of turbulence, because such an average has not been performed in writing the Δf equation; neither Eq. (7) nor Eq. (10) contains a turbulent collision operator. Instead, one should merely coarse-grain over scales much smaller than the collective ones.[90] Because with the rigorous construction (50b) $\Delta\boldsymbol{V}$ does not contain such scales, the averaging of Eq. (54) is trivial:

$$(\partial_t-\hat{L})F_m+\partial_z\cdot(\Delta\boldsymbol{V}F_m)=0. \tag{55}$$

At time $t=0$, F_m describes the initial PDF from which the marker phase-space positions are sampled.

Upon using Eqs. (10) and (55) in Eq. (53), one obtains

$$(\partial_t-\hat{L})w+\partial_z\cdot(\Delta\boldsymbol{V}w)=-p\Delta\boldsymbol{V}\cdot\partial_z\ln f_0+F_m^{-1}S, \tag{56}$$

where $p\doteq f_0/F_m$. Henceforth I shall consider only incompressible flows,[91] in which case the left-hand side of Eq. (56) becomes

$$(\partial_t-\hat{L}+\Delta\boldsymbol{V}\cdot\partial_z)w\equiv Dw/Dt. \tag{57}$$

To evaluate p, note that $p+w=(f_0+\Delta f)/F_m=f/F_m$. Because Eq. (7) (for f) and Eq. (55) (for F_m) are identical in form, it is clear that $F_m=f$ if $F_m(t=0)=f(t=0)$. If one assumes that particular initialization scheme, then $p+w=1$ or $p=1-w$. (More general situations were considered in Ref. 5; see also Ref. 81.) We have thus been led to the fundamental weight equation (written here for $S=0$)

$$\frac{Dw(z,t)}{Dt}=-(1-w)\Delta\boldsymbol{V}\cdot\partial_z\ln f_0\equiv S_0(z,t). \tag{58}$$

Equation (58) is a PDE, just as complicated to solve as is the Δf equation. However, as we have noted, if $\Delta\boldsymbol{V}$ is evaluated by Monte Carlo sampling, then w is merely required at the positions of the markers. Then Eq. (58) becomes the ordinary differential equation (ODE)

$$\dot{w}_i(t)=S_{0,i}(t) \tag{59}$$

that can be time-advanced along with the characteristic equations of motion for the ith marker. This is the fundamental algorithm used in the Δf PIC codes.[92]

Even in the absence of sampling error, the Δf problem involves a complicated, nonlinear, stochastic PDE because of collective turbulent fluctuations, and one should consider $w(z,t)$ to be a random variable to the extent that the equations lead to turbulence. The Monte Carlo sampling procedure introduces additional randomness ("noise"). To call attention to both of those effects, one should in Eq. (58)

replace w and $\Delta \boldsymbol{V}$ by $\tilde{w}$ and $\Delta \tilde{\boldsymbol{V}}$. Then Eqs. (52), (54), and (58) provide the starting point for analytical calculations of the effect of sampling noise. Those are difficult because such noise can mix nonlinearly with the collective fluctuations. A considerable technical complication is that because $\Delta \tilde{\boldsymbol{V}} \sim \tilde{N}_m \tilde{w}$, the previously linear moments of Δf have become quadratically nonlinear. On the positive side, the effects of sampling noise on the ultimate spectral levels may be relatively simple to calculate if it is generated at substantially smaller scales (higher frequencies and shorter wavelengths) than those of the collective turbulence.

To proceed, one must first understand how to treat collective fluctuations in the absence of noise (reviewed in Sec. IV), then consider how those results are modified in the presence of noise (Secs. V and VI). However, it is instructive to immediately examine the special case of stable plasma, which demonstrates a characteristic form for the fluctuation spectrum that will be generalized to include turbulence in the subsequent sections.

4. Near-equilibrium spectrum with sampling noise

Temporarily, let us ignore background gradients that could drive microturbulence and consider the consequences of a small amount of sampling noise on the fluctuation spectrum of a near-equilibrium plasma. In the complete absence of such noise, fluctuations follow from Eq. (10) for Δf, which poses an initial-value problem. However, although arbitrary initial conditions would give rise to transient fluctuations, the time-asymptotic spectrum for stable plasma would vanish.[93]

In the presence of sampling noise of arbitrary size, a complicated self-consistent problem must be solved. However, when the noise is small it can be taken into account perturbatively. Let the bare potential fluctuations associated with the sampling error be called $\delta\breve{\phi}$. To lowest order, $\delta\breve{\phi}$ behaves exactly like an externally imposed "test" potential $\delta\phi^{\text{test}}$. Through linear order, the time-asymptotic total potential in the plasma $\delta\phi^{\text{tot}}$ (including both $\delta\phi^{\text{test}}$ and the induced or polarization response $\delta\phi^{\text{ind}}$) is

$$\delta\phi^{\text{tot}}(\boldsymbol{k},\omega) = \delta\phi^{\text{test}}(\boldsymbol{k},\omega)/\mathcal{D}(\boldsymbol{k},\omega), \tag{60}$$

where $\mathcal{D}(\boldsymbol{k},\omega)$ is the dielectric response function. Thus, to lowest order in $\delta\breve{\phi}$, one can conclude that the time-asymptotic spectrum is

$$\langle \delta\phi\delta\phi\rangle(\boldsymbol{k},\omega) = \frac{\langle \delta\breve{\phi}\delta\breve{\phi}\rangle(\boldsymbol{k},\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2}, \tag{61}$$

where the GK dielectric function is given by Eq. (43).

To calculate the numerator of Eq. (61), one must recall the prescription (52), which can be written as

$$\tilde{M}_s(z,t) \approx \sum_{\bar{s}} \int d\bar{z}\,[F_m(\bar{z},t) + \delta N_m(\bar{z},t)]M_s(z,\bar{z})\tilde{w}(\bar{z},t) \tag{62a}$$

$$= M_s[\Delta\tilde{f}](z,t) + \delta M_s(z,t). \tag{62b}$$

[Equation (51) was used to eliminate w in the first term. The functional notation reminds one that the first term is the usual response of moments such as ϕ to Δf.] When M refers to the ϕ moment, the δM term defines $\delta\breve{\phi}$. In the absence of the $\tilde{w}$ factor in $\delta\breve{\phi}$, the calculation of $\langle \delta\breve{\phi}\delta\breve{\phi}\rangle$ would involve only the properties of δN_m and thus would reduce to the familiar calculation of the fluctuation spectrum due to statistically independent, streaming test markers.[5] Here, however, one must evaluate $\langle (\delta N_m \tilde{w})(\delta N_m \tilde{w})\rangle$. Hu and Krommes argued[5] that this should be approximated by $\langle \delta N_m \delta N_m\rangle\langle \tilde{w}\tilde{w}\rangle$, thus introducing the mean-square weight W. Either the exact or approximate form demonstrates that the Δf sampling noise is reduced by a factor of W from a full-f calculation, which of course was expected from the inception of the Δf algorithm.[24,28]

When fluctuations are unstable,[94] nontrivial time-asymptotic spectra arise even in the absence of any discreteness effects. Heuristically, it is reasonable to expect that Eq. (61) should generalize to a self-consistent balance equation having the form

$$\langle \delta\phi\delta\phi\rangle(\boldsymbol{k},\omega) = \frac{\langle \delta\breve{\phi}\delta\breve{\phi}\rangle(\boldsymbol{k},\omega) + \langle \delta\phi_c\delta\phi_c\rangle(\boldsymbol{k},\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2}, \tag{63}$$

where the subscript c denotes noise due to collective turbulent fluctuations. That is, one expects that the total noise spectrum should appear in the numerator of the spectral balance. Of course, "noise" must be defined precisely and the appropriate (fully nonlinear) form of the dielectric function for turbulence must be determined. I review aspects of that problem in the next section.

IV. TURBULENT FLUCTUATIONS IN CONTINUUM PARTIAL DIFFERENTIAL EQUATIONS

In the last section we saw that fluctuations arise naturally from discreteness (due to either particles or sampling). But they also arise in continuous nonlinear PDEs with smooth initial conditions. This is the traditional arena of analytical turbulence theory. That such equations can spontaneously generate fluctuations (or, more precisely, amplify minute irregularities in initial conditions) is of course known from observations of the physical world. The study of nonlinear dynamics has contributed deep insights through the notion of strange or chaotic attractors;[95] a popular example is the Lorenz system.[96] Such systems typically exhibit exponential sensitivity to small changes in initial conditions. Traditionally that microscopic instability has been dealt with by some sort of statistical averaging, and that is the approach I shall discuss here. Over the years many reviews and some books on the statistical theory of turbulence have appeared.[7,52,97] Here I shall just remind the reader of the basic structure of the equations for spectral balance in nonequilibrium turbulent steady states. That information will be required later when I discuss the incorporation of discreteness effects.

A. Langevin dynamics

A usefully pedagogical and exactly solvable model is the classical Langevin equation[98]

$$\dot{\tilde{v}} + \nu\tilde{v} = \delta a(t), \tag{64}$$

where ν is a constant and δa is traditionally taken to be centered Gaussian white noise. I shall show later that a generalization of such an equation lies at the heart of statistical turbulence theory. Langevin's equation arises from Newton's second law for a test particle, $\dot{v}=a(t)$, by separating the acceleration a into a coherent drag $-\nu v$ and incoherent forcing δa. In a (stable) plasma, the drag term arises because a moving test particle asymmetrically polarizes the surrounding medium, creating a mean electric field that opposes the motion. The incoherent forcing describes the random fields due to all of the other particles. Of course, the assumptions that the drag is linear and that δa is exactly Gaussian are made strictly for convenience.[99] The merit of linear drag is that Eq. (64) can be solved by a Green's function technique. Introduce the *infinitesimal response function* $R(t;t')$ such that

$$\partial_t R(t;t') + \nu R = \delta(t-t'); \tag{65}$$

thus $R(t;t')=H(\tau)e^{-\nu\tau}$ (again, $\tau \doteq t-t'$). Then if $\tilde{v}$ is specified at t_0, the solution of Eq. (64) for $t \geqslant t_0$ is

$$\tilde{v}(t) = \underbrace{R(t;t_0)v_0}_{\langle v|v_0\rangle} + \underbrace{\int_{t_0}^{t} d\bar{t}\, R(t;\bar{t})\,\delta a(\bar{t})}_{\delta v}, \tag{66}$$

which decomposes into a conditional mean $\langle v|v_0\rangle$ and fluctuation δv around that mean. One can eliminate transient effects and the conditional mean by taking $t_0 \to -\infty$; that is appropriate for considering statistically steady states. Thus

$$\delta v(t) = \int_{-\infty}^{t} d\bar{t}\, R(t;\bar{t})\,\delta a(\bar{t}). \tag{67}$$

Define $F(t,t') \doteq \langle \delta a(t)\,\delta a(t')\rangle$. Then the two-time velocity correlation function $C(t,t') \doteq \langle \delta v(t)\,\delta v(t')\rangle$ is obtained from Eq. (67) as

$$C(t,t') = \int_{-\infty}^{t} d\bar{t} \int_{-\infty}^{t'} d\bar{t}'\, R(t;\bar{t})F(\bar{t},\bar{t}')R(t';\bar{t}'). \tag{68}$$

This states that the velocity covariance is determined as a competition between forcing (F) and dissipation (R). If one specializes in white noise, $F(t,t')=2D_v\delta(t-t')$, where D_v is the velocity-space diffusion coefficient. Then, upon using the known forms of $R(\tau)$ and $F(\tau)$, one can perform the integrations required in Eq. (68) to find

$$C(\tau) = (D_v/\nu)e^{-\nu|\tau|}. \tag{69}$$

If one assumes that the fluctuating kinetic energy of the test particle equilibrates on average with the temperature of the medium, i.e., $\frac{1}{2}M\langle \delta v^2\rangle = \frac{1}{2}T$, one finds the well-known Einstein relation $D_v/\nu = T/M$.

If one views R^{-1} as a kind of "dielectric function," then the balance (68) has the same structure as Eqs. (61) or (63). In particular, F plays the role of the covariance of "incoherent noise." Thus the statistical description of the Langevin model adds credibility to the posited form (72). The key lesson to be learned from this model is that the coherent damping ν and the incoherent forcing δa both arise from the same physical effect (here the acceleration of the test particle); one cannot have one without the other, and their sizes are related by energy conservation.

B. Statistical closures for quadratically nonlinear smooth PDEs

Now consider quadratically nonlinear PDEs for a scalar field $\psi(\mathbf{x},t)$. Schematically, those have the form

$$\dot{\psi} = \hat{L}\psi + \tfrac{1}{2}\hat{M}\psi\psi, \tag{70}$$

where $\hat{L}$ and $\hat{M}$ are linear and bilinear operators, respectively. For simplicity, I shall assume that the mean field vanishes,[100] so consider the equation for the fluctuations

$$\delta\dot{\psi} = \hat{L}\delta\psi + \tfrac{1}{2}\hat{M}(\delta\psi\delta\psi - \langle\delta\psi\delta\psi\rangle). \tag{71}$$

Let us assume that this equation gives rise to a dynamics that is extremely sensitive to small changes in initial conditions, so a statistical description is appropriate. Let us also assume that the nonlinear term is energy-conserving in the sense that $\overline{\delta\psi\hat{M}\delta\psi\delta\psi}=0$, where the overline denotes the spatial average. This implies that the nonlinear term cannot behave as a purely positive-definite forcing, so one posits the generalized Langevin form $\frac{1}{2}\hat{M}(\delta\psi\delta\psi - \langle\delta\psi\delta\psi\rangle) = -\int_{-\infty}^{t} d\bar{t}\,\Sigma(t;\bar{t})\,\delta\psi(\bar{t}) + \delta f(t)$, where Σ is at least partly dissipative (it plays the role of a "turbulent collision operator") and δf is a nonlinear forcing analogous to Langevin's δa. The result is

$$(\partial_t - \hat{L})\delta\psi + \int_{-\infty}^{t} d\bar{t}\,\Sigma(t;\bar{t})\,\delta\psi(\bar{t}) = \delta f(t). \tag{72}$$

Such a Langevin equation is not intended to be a mere rewriting of the primitive amplitude Eq. (70); it is at best guaranteed to yield correct results only when statistics are calculated from it. Although the form of Σ and the statistics of δf are unknown at this point, they cannot be totally independent because of the energy-conservation constraint. One anticipates that Σ and δf are functionals of the fluctuation level.

It is not clear that such a Langevin equation can be found. But if it does exist, a Green's-function solution is again useful. Green's function for Eq. (72) obeys

$$\partial_t R(t;t') - \hat{L}R + \int_{-\infty}^{t} d\bar{t}\,\Sigma(t;\bar{t})R(\bar{t};t') = \delta(t-t'). \tag{73}$$

The solution of Eq. (72) thus has the same form as Eq. (67) with δf replacing δa, and the formal inhomogeneous solution for the covariance $C(t,t') \doteq \langle\delta\psi(t)\,\delta\psi(t')\rangle$ is identical to Eq. (68):

$$C = R \star F \star R, \tag{74}$$

where $\star$ denotes time convolution. The fluctuation spectrum is again presented as a balance between nonlinear forcing (F) and linear and nonlinear dissipation ($-\hat{L}+\Sigma$). The great difficulty is that now the nonlinear terms must be allowed to be functionals of C (and R): $\Sigma=\Sigma[C,R]$ and $F=F[C,R]$. Equations (74) and (73) are therefore a complicated transcendental system to be solved for the two-point functions C and R.

Although the existence of the nonlinear Langevin equation may be dubious, it can in fact be shown that the forms of the statistical equations (73) and (74) are completely correct for a very wide class of systems (specifically, those with Gaussian initial conditions; see further discussion of this point in Sec. V). They constitute a system of coupled "Dyson equations" that generalizes Dyson's original work in quantum electrodynamics.[101] This is a profound conclusion from the classical theory of nonequilibrium statistical dynamics, as developed most elegantly by Martin, Siggia, and Rose (MSR).[58] Further details and pedagogical discussion of the MSR procedure with many references can be found in Ref. 7. It is not necessary here to dig deeply into the formalism, but one very important point must be made: *Modern understanding of the classical Dyson equations is very well developed. A large body of knowledge and literature exists that can be tapped and generalized to address problems such as the unification of sampling noise and turbulent fluctuations.*

One famous realization of the Dyson equations is Kraichnan's DIA,[102] which provides specific forms for Σ and F; for details, see Ref. 7. For the DIA, a Langevin model is known.[103,104] As Kraichnan has stressed repeatedly, the mere existence of such an amplitude representation[105] guarantees that statistics calculated from the closure are reasonably behaved, as they must satisfy the infinity of realizability constraints[106,107] that relate to the moments of various orders.

Further reduction leads to a *Markovian statistical closure*. I assume homogeneous statistics, so Eq. (70) can be represented in Fourier space as

$$\partial_t \delta\psi_{\boldsymbol{k}} = L_{\boldsymbol{k}}\delta\psi_{\boldsymbol{k}} + \tfrac{1}{2}\sum_{\Delta} M_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}\delta\psi^*_{\boldsymbol{p}}\delta\psi^*_{\boldsymbol{q}}. \tag{75}$$

Consider the Langevin equation

$$(\partial_t - L_{\boldsymbol{k}})\delta\psi_{\boldsymbol{k}} + \eta^{\mathrm{nl}}_{\boldsymbol{k}}\delta\psi_{\boldsymbol{k}} = \delta f_{\boldsymbol{k}}, \tag{76}$$

where

$$\eta^{\mathrm{nl}}_{\boldsymbol{k}} \doteq -\sum_{\Delta} M_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}M^*_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}}\theta^*_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}C_{\boldsymbol{q}}, \tag{77a}$$

$$\delta f_{\boldsymbol{k}} \doteq \tfrac{1}{2}\widetilde{w}(t)\sum_{\Delta} M_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}(\mathrm{Re}\ \theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}})^{1/2}\widetilde{\xi}^*_{\boldsymbol{p}}\widetilde{\xi}^*_{\boldsymbol{q}}, \tag{77b}$$

$\widetilde{w}(t)$ is centered Gaussian white noise with the unit diffusion coefficient [i.e., $\langle\widetilde{w}(t)\widetilde{w}(t')\rangle=2\delta(t-t')$], and $\widetilde{\xi}_{\boldsymbol{p}}$ and $\widetilde{\xi}_{\boldsymbol{q}}$ are centered random variables (independent of $\widetilde{w}$) whose covariances are to be chosen to agree with $C_{\boldsymbol{p}}(t,t')$ and $C_{\boldsymbol{q}}(t,t')$. The purpose of $\widetilde{w}$ is to ensure that the effect of the forcing is local in time (a technical convenience), i.e., to enforce the Markovian approximation. The quantity $\theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}$ is called the *triad interaction time*. In Eq. (77a) it ensures that $\eta_{\boldsymbol{k}}/k^2$ has the dimensions of $V^2\tau_{\mathrm{ac}}$, and it is required in Eq. (77b) in order to compensate the dimensions of $\widetilde{w}$. Its presence in both of Eqs. (77) is also required on physical grounds to limit the interaction time between distinct Fourier amplitudes. Thus a reasonable definition is $\theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}(t)=\int_{-\infty}^{t}d\bar{t}\,R_{\boldsymbol{k}}(t;\bar{t})R_{\boldsymbol{p}}(t;\bar{t})R_{\boldsymbol{q}}(t;\bar{t})$, where $R_{\boldsymbol{k}}$ is Green's function for the left-hand side of Eq. (76); by time differentiation, one finds the ODE

$$\partial_t\theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}(t) - \Delta L\theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}} + \Delta\eta^{\mathrm{nl}}\theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}} = 1, \tag{78}$$

where, e.g., $\Delta\eta^{\mathrm{nl}} \doteq \eta^{\mathrm{nl}}_{\boldsymbol{k}}+\eta^{\mathrm{nl}}_{\boldsymbol{p}}+\eta^{\mathrm{nl}}_{\boldsymbol{q}}$. Note that if $\mathrm{Im}\,\Delta L\neq 0$ (there are linear waves), θ is complex; thus it is really Re θ that plays the role of a physical interaction time. If the formalism is to be sensible, one must have Re $\theta>0$. Unfortunately, that is not guaranteed for all possible closures;[108] see discussion of realizability in Sec. V A.

One can obtain the equal-time spectral balance that follows from Eq. (76) by noting that $\partial_t|\delta\psi_{\boldsymbol{k}}|^2=2\,\mathrm{Re}(\delta\psi^*_{\boldsymbol{k}}\delta\dot{\psi}_{\boldsymbol{k}})$, multiplying Eq. (76) by $\delta\psi^*_{\boldsymbol{k}}(t)$, performing a formal statistical average, and evaluating $\langle\delta f_{\boldsymbol{k}}(t)\delta\psi^*_{\boldsymbol{k}}(t)\rangle =\int_{-\infty}^{t}d\bar{t}\,\langle\delta f_{\boldsymbol{k}}(t)R^*_{\boldsymbol{k}}(t;\bar{t})\delta f^*_{\boldsymbol{k}}(\bar{t})\rangle$ by noting that $\langle\delta f_{\boldsymbol{k}}(t)\delta f_{\boldsymbol{k}}(t')\rangle =2\delta(t-t')F_{\boldsymbol{k}}(t)$, where

$$F_{\boldsymbol{k}}(t) \doteq \tfrac{1}{2}\sum_{\Delta}|M_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}|^2\ \mathrm{Re}\ \theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}C_{\boldsymbol{p}}(t)C_{\boldsymbol{q}}(t) \tag{79}$$

is positive for Re $\theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}>0$. The final result

$$\partial_t C_{\boldsymbol{k}} = 2(\gamma_{\boldsymbol{k}} - \mathrm{Re}\ \eta^{\mathrm{nl}}_{\boldsymbol{k}})C_{\boldsymbol{k}} + 2F_{\boldsymbol{k}}, \tag{80}$$

where $\gamma_{\boldsymbol{k}}\doteq\mathrm{Re}\,L_{\boldsymbol{k}}$ is the linear growth rate, has exactly the form of the spectral balance equation introduced more heuristically in Sec. I B. Equations (76)–(80) have been called[108] the "DIA-based EDQNM," where EDQNM stands for "eddy-damped, quasinormal, Markovian." The nomenclature correctly implies that this closure is a consistent Markovian reduction of the more-complicated, time-nonlocal, DIA. With the forms (77a) and (79), one can show that the energy-conservation constraint

$$\sum_{\boldsymbol{k}}(-\eta^{\mathrm{nl}}_{\boldsymbol{k}}C_{\boldsymbol{k}} + F_{\boldsymbol{k}}) = 0 \tag{81}$$

is satisfied provided that $M_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}+M_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}}+M_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}=0$. (One can choose a dependent variable such that this is true. Alternatively, one can modify the cyclic constraint to include appropriate weight factors.)

There is a large literature on this closure that cannot be reviewed here; for further discussion and references, see Ref. 7. But it is very useful to make contact with the heuristic spectral balance equation discussed by Kadomtsev,[54] which has been influential within the plasma-physics community. Let I represent the fluctuation energy in the linearly unstable wave numbers $\bar{\boldsymbol{k}}$, $I\doteq\frac{1}{2}\sum_{\bar{\boldsymbol{k}}}C_{\bar{\boldsymbol{k}}}$. Then Eq. (80) can be transcribed to Kadomtsev's Eq. (II.58)[109] as follows:

$$\underbrace{\partial_t C_{\boldsymbol{k}}}_{\partial_t I} \underset{=}{=} \underbrace{2\gamma_{\boldsymbol{k}}C_{\boldsymbol{k}}}_{2\gamma I}\ \underbrace{-\,2\ \mathrm{Re}\ \eta^{\mathrm{nl}}_{\boldsymbol{k}}C_{\boldsymbol{k}} + 2F_{\boldsymbol{k}}}_{-2\alpha I^2}, \quad + q, \tag{82}$$

where α is a positive constant and q represents "the source due to thermal noise." That has so far been omitted from the formalism in this section; it will be discussed in Sec. V. Here, assume that $q=0$ and focus on the nonlinear terms. One sees that the sum of all nonlinear effects is represented by a dissipative term; this requires further discussion. It is true that $\eta_{\boldsymbol{k}}$ must be typically (i.e., for most $\boldsymbol{k}$'s) dissipative, since $C_{\boldsymbol{k}}$ and $F_{\boldsymbol{k}}$ must be positive-definite (see discussion about realizability in Sec. V A) and one has the constraint (81). That the net effect of all nonlinear terms for a linearly unstable wave number should be negative is required in order that a steady state exist.[110] In Kadomtsev's notation, the saturation level is $I=\gamma/\alpha$.

I scales with the total energy content $\mathcal{E}\doteq\frac{1}{2}\Sigma_{\boldsymbol{k}}C_{\boldsymbol{k}}$ of the turbulent spectrum. However, Eq. (82) is not the rigorous evolution equation for $\mathcal{E}$, which is obtained from Eq. (80) with the aid of nonlinear energy conservation as

$$\partial_t\mathcal{E}=2\sum_{\boldsymbol{k}}\gamma_{\boldsymbol{k}}C_{\boldsymbol{k}}. \tag{83}$$

The nonlinear terms are completely absent from this equation. If one represents the right-hand side in terms of an effective growth rate γ_{eff}, then one can write $\partial_t\mathcal{E}=2\gamma_{\mathrm{eff}}\mathcal{E}$. This kind of evolution equation permits no direct determination of $\mathcal{E}$. It states that the spectrum must adjust such that $\gamma_{\mathrm{eff}}=0$ in a steady state, but for multiple wave numbers (there must be at least three, and usually there are many), the single constraint of steady state does not completely fix the spectral distribution $C_{\boldsymbol{k}}$. Instead, one must solve Eq. (80) as a coupled system in all of the $C_{\boldsymbol{k}}$'s, then sum the result over $\boldsymbol{k}$ to obtain $\mathcal{E}$. Obviously a steady state is impossible unless at least one of the $\gamma_{\boldsymbol{k}}$'s is negative (there must be an energy sink somewhere). Entropy considerations[111] suggest that in fact the sum of the $\gamma_{\boldsymbol{k}}$'s should be negative.

Kadomtsev's equation clearly differs in form from Eq. (83). An interpretation of Eq. (82) for positive γ[93] is that it describes the competition between linear excitation and nonlinear *transfer* into stable modes. For negative γ, no steady state is possible unless q is included.[93] I shall further discuss the structure of the spectral balance for nonzero q in Sec. V B 3.

V. TURBULENT FLUCTUATIONS IN KLIMONTOVICH DESCRIPTIONS

We have seen that fluctuations in a many-body plasma arise from both particle discreteness and from nonlinear collective effects that survive even as $\epsilon_p\to 0$. So far, we have considered each of those separately. However, it is important to examine the structure of the theory when both kinds of effect are considered on equal footing. That is interesting in its own right and will also suggest the appropriate generalization to the case of sampling noise, which I shall discuss in Sec. VI.

In fundamental work, Rose[53] derived a renormalized, nonequilibrium theory of the Klimontovich equation that embraces both discreteness and continuum effects. As he stressed, the problem is challenging because of the effects of particle self-correlations, which constrain the fluctuations to be intrinsically non-Gaussian even in the absence of nonlinear effects.

A. Non-Gaussian PDFs and cumulant representations

In this manuscript I shall not require involved technical results on renormalized fluctuation theory. However, it is a goal of this article to emphasize that systematology underlies modern understanding of fluctuation noise. Therefore, I shall include a brief background on the role of cumulant representations in statistical descriptions in order to provide the reader with some perspective on what has (and has not) been accomplished.

The ultimate goal of a statistical formalism is to obtain all relevant properties of a PDF. In many (but not all[112]) cases a PDF $P(x)$ can be constructed from the infinite set of moments $M_n\doteq\langle x^n\rangle$. However, moments do not provide an efficient representation, since the ubiquitous Gaussian PDF $P_G(x)=(2\pi\sigma^2)^{-1/2}\exp\left[-\frac{1}{2}(x-\bar{x})^2/\sigma^2\right]$ can be described by just its mean $\bar{x}$ and standard deviation σ, whereas all even moments of the centered Gaussian exist [and rise exponentially rapidly with order: $M_{2n}=(2n-1)!!\sigma^{2n}$]. Cumulants[113] $C_n\equiv\langle\langle x^n\rangle\rangle$ are defined in such a way that $C_1=\bar{x}$ and $C_2=\sigma^2$; thus for a Gaussian $C_{n\geqslant 3}=0$. For a nearly Gaussian PDF, one may hope that the higher-order cumulants are small and calculable with the aid of perturbation theory. That is the case for a weakly coupled plasma, for example, provided that one restricts attention to time and space scales of the order of the plasma period and Debye length, respectively.

Moments are the coefficients in the Taylor expansion of the characteristic function $Z(k)\doteq\langle e^{-ikx}\rangle$ if that expansion exists. (Note that Z is the Fourier transform of the PDF.) One has formally $Z(k)=\Sigma_{n=0}^{\infty}M_n(-ik)^n/n!$. Cumulants C_n are analogously defined as the coefficients in the formal expansion of $\ln Z$: $\ln Z(k)=\Sigma_{n=1}^{\infty}C_n(-ik)^n/n!$. Properties of the logarithm enable one to prove a general formula relating M_n to cumulants of order n and below. The rule is to partition the n factors comprising M_n into all possible subsets, then to assign a cumulant to each subset.[114] Thus, e.g.,

$$M_1=C_1, \tag{84a}$$

$$M_2=C_1^2+C_2, \tag{84b}$$

$$M_3=C_1^3+3C_1C_2+C_3, \tag{84c}$$

$$M_4=C_1^4+4C_1C_3+6C_1^2C_2+3C_2^3+C_4. \tag{84d}$$

Truncated cumulant expansions are generally not *realizable*, i.e., they do not obey the infinity of constraints between cumulants of various orders that follow from the positive-definiteness of the PDF.[106] However, if a statistical closure model is the exact description of a stochastic amplitude model,[115] then realizability is guaranteed. The conventional EDQNM is, in fact, not realizable in the presence of linear waves[116] because the Re $\theta_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}$ that appears in Eqs. (77b) and (79) can be transiently negative and then does not make sense as a modal interaction time. Bowman, Krommes, and Ottaviani[108] discussed a *realizable Markovian closure* that cured that problem and was shown to be quantitatively successful.[117–119]

B. Non-Gaussian initial conditions and the Klimontovich representation

It is well known that the renormalized closures discussed in Sec. IV, such as the DIA or EDQNM, are incorrect in the presence of non-Gaussian initial conditions.[120] This can be understood by realizing that non-Gaussian initial conditions

$C_{n\geq 3}(0)$ should logically affect the statistical evolution of the two-point correlation function $C \equiv C_2$, yet no such terms are evident in the DIA (or even in the more complete, vertex-renormalized[58]) spectral evolution equation for C. For continuum PDEs, that is frequently not too worrisome because one expects that steady-state statistics should forget the details of initial conditions in the infinitely remote past. However, as Rose emphasized, this argument fails in the presence of discrete particle self-correlations. Thus, let us consider the first few cumulants of the Klimontovich microdensity. I shall use C_n for the conventional n-particle correlation functions as introduced in kinetic theory [e.g., $C_1(1)=f(1)$ and $C_2(1,2)=g(1,2)$, g being the pair correlation function] and the double-bracket notation for the Klimontovich cumulants. At equal times, one has (considering a single species for simplicity)

$$\langle\langle \widetilde{N}(1,t)\rangle\rangle = C_1(1,t), \tag{85a}$$

$$\langle\langle \widetilde{N}(1,t)\widetilde{N}(2,t)\rangle\rangle = \bar{n}^{-1}\delta(1-2)C_1(1,t) + C_2(1,2,t), \tag{85b}$$

$$\begin{aligned}\langle\langle \widetilde{N}(1,t)\widetilde{N}(2,t)\widetilde{N}(3,t)\rangle\rangle &= \bar{n}^{-2}\delta(1-2)\delta(1-3)C_1(1,t)\\ &\quad + \bar{n}^{-1}[\delta(1-2)C_2(2,3,t) + \text{c.p.}]\\ &\quad + C_3(1,2,3,t)\end{aligned} \tag{85c}$$

(c.p. means cyclic permutations). Even in the absence of three-particle correlations ($C_3=0$), the three-point Klimontovich cumulant is nonvanishing because of particle self-correlations. This remains true as $t\to\infty$.

1. The renormalized equations of Rose

In principle, the self-correlation effects can be of arbitrary size. In spite of that, Rose was able to obtain a formally correct system of renormalized equations that treated the self-correlations on equal footing with continuum nonlinear effects. His elegant method was to apply the Schwinger variational formalism [previously used by MSR (Ref. 58) to derive renormalized equations for continuum PDEs; see Ref. 7 for discussion and further references] to the occupation-number representation of Doi.[121] Most of the details do not concern us (although it is interesting that Rose was forced to consider the renormalization of a cubically nonlinear equation even though the Klimontovich equation is merely quadratic). However, the form of the result is important. It is quite general in formal renormalizations that the second-order statistics are presented in the form of coupled Dyson equations[101] for an infinitesimal response function R and a two-point correlation function C. In a notation somewhat altered from that of Rose, the Dyson equations are the straightforward generalization of Eqs. (73) and (74) to include phase-space indices:

$$(\partial_t - \hat{L})R(z,t;z',t') - \int_{t'}^{t} d\bar{t}\int d\bar{z}\,\Sigma_{-+}(z,t;\bar{z},\bar{t})R(\bar{z},\bar{t};z',t') = \delta(z-z')\delta(t-t'), \tag{86a}$$

$$(\partial_t - \hat{L})C(z,t,z',t') - \int_{-\infty}^{t} d\bar{t}\int d\bar{z}\,\Sigma_{-+}(z,t;\bar{z},\bar{t})C(\bar{z},\bar{t},z',t') = \int_{-\infty}^{t'} d\bar{t}\int d\bar{z}\,\Sigma_{--}(z,t,\bar{z},\bar{t})R(z',t';\bar{z},\bar{t}). \tag{86b}$$

(The significance of the spinor-index subscripts on the Σ's is explained by Rose.) In general, the Σ's are determined by closed but highly nontrivial functional equations, and extracting specific results from this system is extremely formidable. However, it is noteworthy that the singular term in Eq. (85b) involves a factor of $\bar{n}^{-1}$, i.e., it is $O(\epsilon_p)$. This term and the similar terms in Eq. (85c) are therefore small for weak coupling. This motivates a perturbative expansion of the renormalized equations that determine the Σ's. Rose worked out the necessary relations through second order in the coupling. He called the result the *particle direct-interaction approximation* (PDIA) because when discreteness effects are ignored the approximation correctly reduces to the Vlasov DIA studied by DuBois and Espedal,[122] Krommes,[7,123] and others (see references in Ref. 7).

Note that Rose's specific results for the Σ's are correct for the standard, quadratically nonlinear Klimontovich equation. Since, as we have seen, sampling noise in the Δf algorithm leads to a cubically nonlinear equation (the self-consistent field term scales as $\widetilde{N}\widetilde{w}\Delta\widetilde{f}$), one cannot immediately apply all of Rose's formulas to the calculation of Δf statistics. Although one can contemplate renormalizing a cubically nonlinear system that includes discreteness, the details are rather tedious and I shall not attempt it here. Instead, I shall just briefly discuss the structure of Rose's Klimontovich results. In Sec. VI I shall apply those insights to the Δf system in the limit of small sampling noise.

2. Recovery of the weakly coupled fluctuation spectrum

A basic exercise is to verify that one can recover from Rose's results the familiar formula (33) for the weakly coupled fluctuation spectrum of a many-body system. That is not entirely immediate and was not discussed explicitly by Rose. First, one must recognize that the two-point Klimontovich cumulant $\langle \delta N(t)\delta N(t')\rangle$ and the pair correlation function $C(t,t')$ are distinct entities. At equal times, we have already seen that to be the case from Eq. (85b). Rose gave the generalization to unequal times [his Eq. (71) rewritten to emphasize causality]:

$$\begin{aligned}\langle \delta N(1,t_1)\delta N(2,t_2)\rangle_+ &= R(1,t_1;2,t_2)\bar{n}_2^{-1}f(2,t_2)\\ &\quad + C_+(1,t_1,2,t_2)\\ &\quad + G_+(1,t_1;2,t_2^+;2,t_2),\end{aligned} \tag{87}$$

where the subscript $+$ denotes a one-sided function $[A_+(t,t') \doteq H(t-t')A(t,t')]$ and G is a certain three-point cumulant. G can be shown to vanish at equal times, so Eq. (87) correctly reduces to Eq. (85b).[124]

Second, one requires the result that through first order in the weak coupling

$$\Sigma_{--}(1,t_1,2,t_2) = \delta(t_1-t_2)\boldsymbol{\epsilon}(\boldsymbol{x}_1-\boldsymbol{x}_2)(\bar{n}q)_2\cdot\boldsymbol{\partial}_1 \times[f(1,t_1)f(2,t_2)+C(1,t_1,2,t_2)] + (1\Leftrightarrow 2), \tag{88}$$

where $\boldsymbol{\epsilon}(\boldsymbol{x})$ is the field due to a unit charge at the origin. [This is Rose's Eq. (72) in my notation.] Finally, it is a well-known property of the response function R that, if $\hat{\boldsymbol{\mathcal{E}}}$ is the linear operator that constructs the electric field from the distribution function, i.e., $\boldsymbol{E}=\hat{\boldsymbol{\mathcal{E}}}f$ or $\boldsymbol{E}(\boldsymbol{x},t)=\Sigma_{\bar{s}}(\bar{n}q)_{\bar{s}}\int d\bar{z}\,\boldsymbol{\epsilon}(\boldsymbol{x}-\bar{\boldsymbol{x}})f_{\bar{s}}(\bar{z},t)$, then

$$\hat{\boldsymbol{\mathcal{E}}}R = \mathcal{D}^{-1}\hat{\boldsymbol{\mathcal{E}}}g, \tag{89}$$

where g is the renormalized single-particle propagator.[7,53,122] These facts are combined in Appendix D to show that one indeed recovers Eq. (33) when g is replaced by the zeroth-order propagator $g^{(0)}$ and $\mathcal{D}$ is replaced by the Vlasov dielectric function $\mathcal{D}^{(0)}$.

3. Structure of the particle direct-interaction approximation: A modified Kadomtsev equation

In the last section, we saw that discreteness noise in stable plasma is captured by the first-order term in the weak-coupling expansion. At second order, one finds all of the mode-coupling effects contained in the Vlasov DIA (which in turn can be shown to contain the physics of conventional fluid renormalizations[7]) as well as additional contributions due to discrete particle noise. The expressions for the Σ's [Rose's Eqs. (78) and (79)] are involved and will not be written or discussed here in detail. (To my knowledge, little or no work has been done on the consequences of those formulas.) However, one may use the general structure of the equations to argue for the form of a heuristic spectral balance equation that smoothly connects the stable, near-equilibrium state with the turbulent nonequilibrium state that emerges as the background gradient is raised from zero. Kadomtsev proposed such an equation, as discussed in Sec. IV B. I shall argue for a slightly different but closely related form.

Kadomtsev's spectral balance equation is [repeating Eq. (82) here for convenience]

$$\partial_t I = 2\gamma I - 2\alpha I^2 + q, \tag{90}$$

where q represents the thermal noise and γ presumably represents the typical linear growth rate of a collective instability. Kadomtsev correctly noted that for sufficiently negative γ the steady-state balance in his equation is between the linear damping and the noise, $I\approx q/(2|\gamma|)$. However, this indicates a subtle problem with Eq. (90), because excitation due to particle discreteness should exist even in the complete absence of a collective mode ($\gamma\to-\infty$). It is true that q can be calculated from the balance between Cerenkov emission and Landau damping, but the Landau damping rate for discreteness-related fluctuations need have nothing to do with the growth rate of, say, a drift wave. However, Kadomtsev's equation does capture the tendency for small thermal fluctuations to be amplified in the vicinity of marginal instability; the estimate $I\approx q/(2|\gamma|)$ diverges as $\gamma\to 0$.

In principle, one can derive a Kadomtsev-type equation from the rigorous spectral balance equation of the renormalized theory. The results from Appendix D show that the steady-state spectral balance equation has the form

$$S_{\boldsymbol{k}}(\omega) = \frac{N^{(1)}(\boldsymbol{k},\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2} + \frac{N^{(2)}(\boldsymbol{k},\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2}, \tag{91}$$

where I use S to denote the velocity-integrated C, $N^{(1)}$ is the numerator of Eq. (33) [not merely $\propto \Sigma_{--}^{(1)}$], and $N^{(2)} \doteq \hat{\boldsymbol{\mathcal{E}}}(g\Sigma_{--}^{(2)}g^{\dagger})\hat{\boldsymbol{\mathcal{E}}}^{\dagger}$. The goal is to integrate Eq. (91) over all frequencies and sum it over all wave numbers, thereby deducing a qualitatively correct and self-consistent equation for the spectral intensity $I\doteq\Sigma_{\boldsymbol{k}}(2\pi)^{-1}\int d\omega\, S_{\boldsymbol{k}}(\omega)$. Thus, one needs to understand the S dependence of $N^{(2)}$. Note from Eqs. (D1) and (D2) that $S=O(R\bar{n}^{-1}f,C)$, where the notation $O(x,y)$ means $O(ax+by)$ for constant a and b. Examination of Rose's Eq. (79) shows that $\Sigma_{--}^{(2)}=O(C^2,R\bar{n}^{-1}fC)$. If one ignores terms of $O(\bar{n}^{-2})$, one can therefore argue very roughly that $\Sigma_{--}^{(2)}=O(S^2)$. This is the same scaling with intensity as in the Vlasov and fluid DIA, now generalized to include the effects of particle discreteness. Of course, it is an extremely rough estimate that ignores considerable kinetic detail. It is not true, for example, that either S or Σ_{--} are literally functionals of the sum $R\bar{n}^{-1}f+C$. Such functional dependence should not be expected because of the complicated form of the nonlinear dielectric function: it is built not from f alone but from $\bar{f}\doteq f+O(C)$.[7,122]

In Eq. (91), the fully renormalized dielectric function appears. For considering linear instability or even stable fluctuations close to marginality, renormalization is essential because nonlinear damping must always overwhelm linear growth if a steady-state balance with the nonlinear forcing is to be achieved. Obviously one cannot calculate the frequency integral of Eq. (91) in detail without very considerably more work. But one can attempt to extract basic scaling information by assuming a nearly resonant form for $\mathcal{D}(\boldsymbol{k},\omega)$. Thus, let us assume the presence of weakly damped Ω_H modes, whose contributions to the $N^{(1)}$ term produce the standard discreteness spectrum as well as a drift wave $\omega=\Omega_*$ that can be varied from large damping rate through marginal stability to large growth rate by varying a parameter. It is important that the same denominator $|\mathcal{D}|^2$ appears in both terms of Eq. (91). Thus each of the $N^{(1)}$ and $N^{(2)}$ terms receives contributions from *both* Ω_H and Ω_*, in principle.

Integrating the $N^{(1)}$ term over the Ω_H modes produces the usual discreteness spectrum, which I call here I_0,

$$I_0 = \int_{\Omega_H}\frac{d\omega}{2\pi}\frac{N^{(1)}(\boldsymbol{k},\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2}. \tag{92}$$

This provides a small base level of fluctuations. Note that I_0 is not quite the same as q, the latter having the dimensions of $\gamma_* I_0$ for some rate γ_*.

Next, let us integrate the $N^{(2)}$ term over the drift wave. For positive growth rate γ, one may use formula (27) with the turbulent damping η replacing $|\gamma|$. Even as γ is reduced to zero, a certain level of nonlinear damping must persist; there can be no zero of $\mathcal{D}$ on the real ω axis in a steady state.

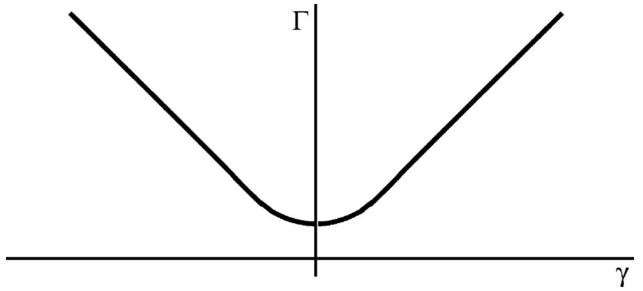

FIG. 4. Qualitative dependence of the nonlinear broadening rate Γ on linear growth rate γ. The broadening becomes small in the vicinity of marginal stability and tracks $|\gamma|$ as $|\gamma|\to\infty$.

As $\gamma\to-\infty$ the contribution from the drift wave should vanish. One can capture all of this behavior by approximating [cf. Eq. (27)]

$$\frac{1}{|\mathcal{D}(\boldsymbol{k},\omega)|^2} \approx \frac{1}{|\mathcal{D}'|^2}\frac{1}{\Gamma}\pi\delta(\omega-\Omega_*), \tag{93}$$

where $\Gamma(\gamma)$ is a positive function whose dependence on γ is sketched in Fig. 4. Then the Ω_* contribution to the $N^{(2)}$ term takes the form $\alpha_2 I^2/\Gamma$, where α_2 is a constant. [Note that α_2 is not quite the same as Kadomtsev's α: α_2 describes the level of incoherent scattering, whereas α describes the net nonlinear effect including coherent turbulent damping. See the discussion in the vicinity of Eq. (99) below.]

We have yet to discuss the Ω_* contribution to the $N^{(1)}$ term and the Ω_H contribution to the $N^{(2)}$ term. First, however, consider what we have achieved so far, which is the steady-state balance

$$I = \epsilon I_0 + \alpha_2 I^2/\Gamma, \tag{94}$$

where I have inserted an ϵ in front of the discreteness term to remind us that it is small. Equation (94) can be rewritten as the quadratic equation

$$\alpha_2 I^2 - \Gamma I + \epsilon\Gamma I_0 = 0. \tag{95}$$

Of course, this can be solved exactly, but it is more instructive to analyze it qualitatively from the point of view of asymptotic balances. Those can be conveniently visualized by Kruskal diagrams,[125,126] in which powers of the asymptotic parameter ϵ are plotted against powers of the dependent variable I, then lines are brought up from below to rest on the lowest-lying points. Those lines then connect the terms that are in dominant asymptotic balance. To analyze Eq. (95), one needs to order Γ with ϵ. First consider $\Gamma = O(1)$. The associated Kruskal diagram is shown with solid lines in Fig. 5. It shows one balance between the terms of $O(I^1)$ and $O(I^0)$, dominantly $I=\epsilon I_0$. The other balance is between the terms of $O(I^1)$ and $O(I^2)$: $I=\Gamma/\alpha_2$. These are the two limiting cases we expect: a "laminar" solution with just discreteness noise, and a turbulent solution. The latter is the turbulent balance discussed by Kadomtsev if one writes $\Gamma = O(\gamma)$ and $\alpha_2 = O(\alpha)$.

It is, however, troubling that the spectral balance equation has provided two solutions, since it is unclear which one to choose. One expects that as the drift-wave growth rate is

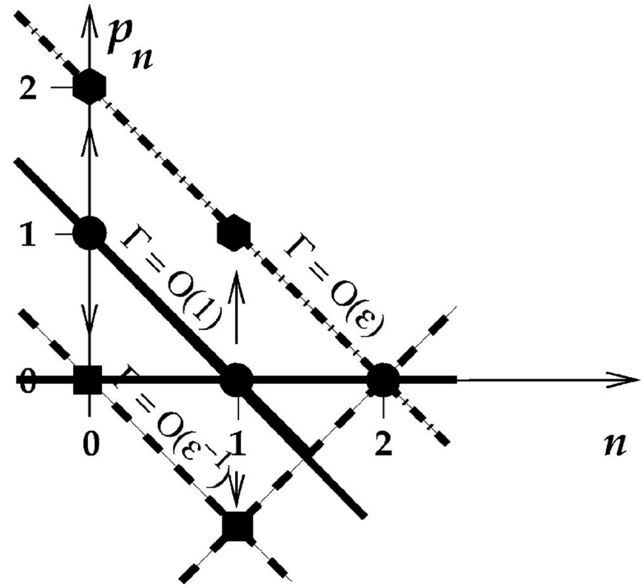

FIG. 5. Kruskal diagrams for the dominant balances in the spectral balance Eq. (95), for various orderings of Γ with ϵ. Powers n of the dependent variable I are plotted on the abscissa; powers p_n of ϵ are plotted on the ordinate. The point at (2,0) remains fixed while the $n=0$ and $n=1$ points move up or down as the ordering of Γ with ϵ is varied, maintaining a $-45°$ slope. The dashed-dotted line corresponding to $\Gamma = O(\epsilon)$ describes the crossover point at which all three terms are in balance and the stable physical solution may switch from one root to the other.

varied from $-\infty$ to $+\infty$ the spectral level should begin at the discreteness level ϵI_0 and, as γ passes through 0, transition to the driven state with $I=\gamma/\alpha$. Thus let us consider $\Gamma(\gamma)$ and inquire for what ordering all three terms of Eq. (95) are in balance; that is where a transition between roots can occur. As Γ is varied as a function of ϵ, the points associated with I^0 and I^1 move up or down while keeping their relative orientation of $-45°$. Clearly all three terms balance when $\Gamma = O(\epsilon)$ (the dashed-dotted line of Fig. 5). This denotes a point of bifurcation at which stability of the two solutions flips and the stable solution crosses from one root to the other.

If one accepts that the limits are correct, the role of the cross terms [the integrations of the $N^{(1)}$ term over Ω_* and the $N^{(2)}$ term over Ω_H] must be to refine the transition between regimes. Note that when a collective mode is brought to marginal stability, a kind of critical opalescence ensues; that intermediate regime is very difficult to treat.[127] To explore it quantitatively would require an exceedingly involved calculation that I shall not attempt.

I can, however, suggest a modified Kadomtsev equation that correctly captures the expected qualitative behavior. Let ΔI be the difference between the total fluctuation level and the discreteness noise, $\Delta I \doteq I - I_0$ (I now drop the ϵ). Then heuristically replace I^2 by ΔI^2 in Eq. (94), $\Delta I = \alpha_2 \Delta I^2/\Gamma$. This has the exact roots

$$\Delta I = 0, \tag{96a}$$

$$\Delta I = \Gamma/\alpha_2. \tag{96b}$$

The associated spectral evolution equation is

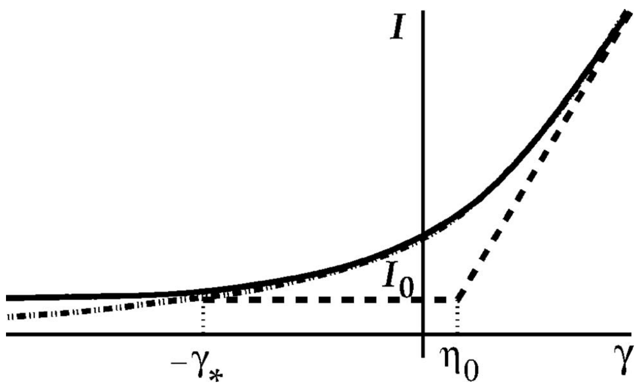

FIG. 6. Behavior of saturated intensity as a function of growth rate. Dashed line: piecewise-linear model; dashed-dotted-dotted line: Kadomtsev's prediction; solid line: smooth interpolation of the piecewise-linear model.

$$\frac{1}{2}\frac{\partial \Delta I}{\partial t} + \Gamma \Delta I = \alpha_2 \Delta I^2. \tag{97}$$

To understand the predictions of Eq. (97), imagine varying γ for fixed I_0. One needs a specific form for the nonlinear damping $\Gamma(\gamma)$. That follows from renormalized theory in the form of the Σ_{-+} term, which as shown by Rose has the same degree of complexity as does Σ_{--}, i.e., $\Sigma_{-+}=O(R\bar{n}^{-1}f,C)$. Σ_{-+} also scales with the triad interaction time θ, which exhibits various scalings with spectral intensity depending on the strength of the turbulence. For purposes of illustration, I shall adopt the quasilinear ordering and assume that Σ_{-+} can be written as the sum of a small reference, discreteness-induced broadening rate η_0 (Ref. 128) and a collective-turbulence-induced rate $\eta^{\mathrm{nl}} \doteq \alpha_1 \Delta I$. Thus

$$\Gamma(\gamma) = -\gamma + \eta_0 + \alpha_1 \Delta I. \tag{98}$$

The solution to Eq. (96b) is then readily found to be

$$\Delta I = (\gamma - \eta_0)/\alpha, \tag{99}$$

where $\alpha \doteq \alpha_1 - \alpha_2$ ($\alpha > 0$ for consistency). It is straightforward to analyze Eq. (97) for the linear stability of the roots (96a) and (99). Assuming that perturbations vary as $e^{\lambda t}$, one finds

$$\Delta I = 0: \quad \lambda = 2(\gamma - \eta_0), \tag{100a}$$

$$\Delta I = (\gamma - \eta_0)/\alpha: \quad \lambda = -2(\gamma - \eta_0). \tag{100b}$$

Thus for $\gamma < \eta_0$ one must select the stable $\Delta I=0$ root, which describes the base level of discreteness noise. For $\gamma > \eta_0$, the turbulent root is stable and the solution asymptotes to the Kadomtsev solution $I \to \gamma/\alpha$. This piecewise-linear behavior is graphed in Fig. 6, where it is also contrasted with Kadomtsev's original prediction. To normalize the two predictions, I have chosen $q=\gamma_* I_0$ [$\gamma_*=O(1)$ and $\eta_0=O(\epsilon)$] so that Kadomtsev's solution intersects $I=I_0$ for $\gamma \approx -\gamma_*$. Kadomtsev's curve correctly smooths out the piecewise-linear approximation, interpolating between negative and positive γ and showing the amplification of the thermal level in the vicinity of marginal stability (effects presumably captured by the cross terms that have been omitted in the integration of the spectral balance). In essence, the two models differ only in their behavior for large negative γ, for which Kadomtsev predicts no fluctuations at all whereas the present model asymptotes to the discreteness level. This minor difference is inessential for discussing the level of fluctuations far above threshold.

In discussing interpolations of the spectral level in the vicinity of marginal stability, one should note that, in detail, it matters at what frequency the discreteness noise is emitted, even though the usual spectral balance equation for $C_k(t)$ merely describes the total energy in a given $\boldsymbol{k}$, integrated over all frequencies. If discreteness noise resides in high-frequency stable normal modes, while the collective instability is at low frequency, the interaction between them should be highly nonresonant and there should be little effect on the collective mode. This is the behavior observed by Jenkins and Lee[47] in their simulations of a simple model.

Whether or not marginal amplification exists, it is more relevant to consider behavior on the turbulent branch. For the turbulent solution (99), the total broadening rate is readily evaluated to give

$$\Gamma = \left(\frac{\alpha_2}{\alpha}\right)(\gamma - \eta_0). \tag{101}$$

For $\gamma < \eta_0$, the solution switches to the $\Delta I=0$ branch and $\Gamma = -\gamma + \eta_0$. Thus for the piecewise-linear model

$$\Gamma(\gamma) = |\gamma - \eta_0| \begin{cases} 1 & (\gamma \leqslant \eta_0) \\ \alpha_2/\alpha & (\gamma \geqslant \eta_0), \end{cases} \tag{102}$$

in qualitative agreement with Fig. 4.

On the turbulent branch, Γ varies monotonically with γ, which is intuitively reasonable. However, another frequently voiced belief is that the effect of discreteness noise should be to increase the total broadening.[129] Although that is true on the laminar branch, it is contradicted by formula (101) for the turbulent branch, which decreases as η_0 is increased for fixed γ. This behavior occurs because η_0 opposes the linear forcing. The net forcing $\gamma - \eta_0$ then sets the size of the nonlinear transfer, which is related to the net size of the turbulence-induced nonlinearity and ultimately determines the total broadening. (If α_2 were set to zero, that broadening would vanish. That unphysical result is the implicit prediction of the early resonance-broadening theory of Dupree.[7,130,131]) That Γ vanishes for $\gamma = \eta_0$ is due to the overly simplistic piecewise-linear model; it remains positive in a Kadomtsev-type interpolation.

I stress that the new spectral evolution equation (97) has not been derived rigorously. The validity of the detailed consequences derived from there is therefore uncertain. My goals have been to (i) demonstrate that there is no inherent contradiction in the possibility that enhancing discreteness noise may lead to decreased turbulent broadening, and (ii) elucidate the minimal level of complexity faced by anyone who would attempt analytical estimates of spectral balances in the face of arbitrary noise sources. That complexity is nontrivial, no matter how simple various heuristic guesses might appear to be. There is clearly room for considerable further work. However, it would appear that, as for so many other topics, Kadomtsev correctly distilled the essence of the behavior.

4. Turbulent broadening and turbulent flux

A basic goal of numerical simulation and analytical theory is calculation of the flux Q that appears in the continuity equation $\partial_t\langle\psi\rangle+\partial_x Q=0$ (here written in the absence of external sources) for the mean (background) field $\langle\psi\rangle$ ($\psi=n$ or T). Even given a basic understanding of spectral balance, it is nontrivial to determine Q. The problem is that Q requires cross correlations such as $\langle\delta V_{E,x}\delta T\rangle$, whereas the analyses of the spectral balance I have given so far focus merely on turbulent intensities. One popular way of sidestepping this issue invokes the quasilinear approximation, wherein the requisite phase relations are extracted from linear theory. An entire industry has been developed here, but a review thereof is beyond the scope of this article.

In lieu of rigorous solutions for cross correlations, an alternate approach more in the spirit of nonlinear turbulence theory is to write $Q=-D\partial_x\langle\psi\rangle$, then estimate D from the mean infinitesimal response. This is an approximation because for nonlinear problems incremental and steady-state transport coefficients are distinct entities. However, although their values will surely be numerically different, one may hope that they at least share common scalings. Now mean infinitesimal response is nothing but the dynamics of the response function R. Therefore I consider the long-wavelength limit of the fluctuation-induced contributions to $\Gamma(\gamma)$ and write them in diffusive form, i.e., proportional to k^2. In principle, the results of the spectral sums implicit in the η's may differ depending on the source of the fluctuations. Following Ref. 1, I postulate that the discreteness noise gives rise to isotropic diffusion while I allow for the possibility that the contribution from collective turbulence is anisotropic; thus

$$\eta_0+\eta^{\mathrm{nl}}=k^2D_0+k_r^2D^{\mathrm{nl}}, \tag{103}$$

where $k^2\doteq k_r^2+k_\theta^2$. The left-hand side of Eq. (103) can be calculated from the piecewise-linear model to be $f_1\gamma-f_2\eta_0$, where $f_i\doteq\alpha_i/\alpha$. The macroscopic diffusion coefficient D is now asserted to be the sum of D_0 and D^{nl}, which can be easily found to be

$$D=D_0+D^{\mathrm{nl}}=f_1\left(\frac{\gamma}{k_r^2}\right)-\left(\frac{k_\theta^2}{k^2}+f_2\right)\left(\frac{\eta_0}{k_r^2}\right). \tag{104}$$

This predicts that D decreases as η_0 increases. Note that the effect exists for $f_2=0$ (incoherent noise neglected) and is enhanced for the physical situation with $f_2>0$. Furthermore, it persists even for $k_\theta=0$ if $f_2>0$. The reduction arises as the consequence of balances involving the integrated spectral level, and is thus robust. It is not, for example, related to some sort of subtle modification of a kinetic resonance that might affect the basic size of γ. It is a generic property of energy-conserving nonlinear mode coupling in the face of the competition between linear growth and noise-induced damping.

VI. NONEQUILIBRIUM SPECTRAL BALANCE WITH ΔF-PIC SAMPLING NOISE

The discussion of the previous section focused on the role of noise due to discrete particles. I now consider the consequences of sampling noise in the Δf algorithm. Formally, the problem can be posed as the calculation of the statistical properties of the smooth Δf (or w) equation coupled to the discrete Klimontovich marker equation. As we have seen above, the coupling is cubic and formidable to renormalize in all generality. However, Hu and Krommes[5] showed that one can make progress when the discreteness effects are small.

Hu and Krommes pointed out that in the presence of sampling error two kinds of shielding effects occur. First, there is the conventional process whereby any bare fluctuation (from either turbulent mode coupling or sampling error) is shielded by the full dielectric function $\mathcal{D}$ of the turbulent medium (considered to be smooth). Second, the discrete marker positions are perturbed by the presence of sampling error and will respond such that the error is reduced. This latter effect (also a kind of shielding) is small in the Δf algorithm because the size of the Klimontovich fluctuation is weighted by w.

To be more quantitative, I consider the Δf equation in the presence of sampling error (denoted by a breve accent):

$$(\partial_t-\hat{L})\Delta\tilde{f}+\partial_z\cdot[(\Delta\tilde{\boldsymbol{V}}+\Delta\breve{\boldsymbol{V}})\Delta\tilde{f}]=0. \tag{105}$$

Here $\Delta\tilde{\boldsymbol{V}}$ is a linear functional of $\Delta\tilde{f}$, $\Delta\breve{\boldsymbol{V}}=O(\delta N_m\tilde{w})$ is the second term of Eq. (62b) and the source of sampling error in Eq. (105), and the tilde denotes randomness due to (only) the sampling error (not collective turbulence). One may write $\Delta\tilde{f}=\Delta\bar{f}+\Delta f'$, where the overline denotes an average over the sampling noise. To obtain the marker fluctuations δN_m, one may begin with the Klimontovich-type equation

$$(\partial_t-\hat{L})\tilde{N}_m+\partial_z\cdot[(\Delta\tilde{\boldsymbol{V}}+\Delta\breve{\boldsymbol{V}})\tilde{N}_m]=0. \tag{106}$$

The equation for the smooth marker distribution F_m follows by averaging Eq. (106) over *just the microscopic noise*:

$$(\partial_t-\hat{L})F_m+\partial_z\cdot(\Delta\bar{\boldsymbol{V}}F_m)+\partial_z\cdot\overline{(\Delta\boldsymbol{V}'\,\delta N_m)}+\partial_z\cdot\overline{(\delta\breve{\boldsymbol{V}}\delta N_m)}$$
$$=0, \tag{107}$$

where $\Delta\bar{\boldsymbol{V}}\doteq\Delta V[\Delta\bar{f}]$. The last term of Eq. (107) is analogous to the plasma collision operator; I shall neglect it by assuming that the noise is sufficiently small. To understand the term in $\Delta\boldsymbol{V}'$, one must return to Eq. (105), which decomposes into

$$0=\underline{(\partial_t-\hat{L})\Delta\bar{f}+\partial_z\cdot(\Delta\bar{\boldsymbol{V}}\Delta\bar{f})}+\partial_z\cdot\overline{(\Delta\boldsymbol{V}'\Delta f')}$$
$$+\partial_z\cdot\overline{(\delta\breve{\boldsymbol{V}}\Delta f')}, \tag{108a}$$

$$0=(\partial_t-\hat{L})\Delta f'+\underline{\partial_z\cdot(\Delta\bar{\boldsymbol{V}}\Delta f')}+\partial_z\cdot(\Delta\boldsymbol{V}'\Delta\bar{f})$$
$$+\partial_z\cdot(\delta\breve{\boldsymbol{V}}\Delta\bar{f}+\cdots), \tag{108b}$$

where quadratic fluctuation terms have not been written explicitly and will be assumed to be negligible. The underlined term involves velocity fluctuations due to collective turbulence and behaves as a random correction to the linear propagator. Thus $\Delta f' \approx -R\partial_z \cdot (\delta\check{V}\Delta\bar{f})$, where R is a Vlasov-type response function (including velocity fluctuations due to the microturbulence). R describes how the sampling error due to $\Delta\check{\boldsymbol{V}}$ is shielded by the dielectric properties $\mathcal{D}$ of the turbulent medium to give rise to the observable noise $\Delta f'$. Since $\Delta f' = O(\delta\check{V})$, the third term of Eq. (107) is negligible as well. Finally, the Klimontovich fluctuation obeys

$$(\partial_t - \hat{L})\delta N_m + \underline{\partial_z \cdot (\Delta\bar{\boldsymbol{V}}\delta N_m)} + \partial_z \cdot (\Delta \boldsymbol{V}' F_m) + \partial_z \cdot (\delta\check{\boldsymbol{V}} F_m) + \cdots . \tag{109}$$

Although this equation is similar in form to Eq. (108b), a fundamental difference is that $\Delta\boldsymbol{V}' = O(\Delta\check{\boldsymbol{V}}) = O(\delta N_m w)$. This term is related to the second, marker-shielding effect mentioned above and will be neglected because of the extra factor of w.

With the $\Delta\boldsymbol{V}'$ and $\Delta\check{\boldsymbol{V}}$ terms neglected in Eq. (109), we see that the test markers essentially propagate undisturbed, exactly as discrete physical particles do at lowest order [cf. Eq. (32)]. It is here that one makes the connection to the general structure of Rose's renormalized equations for discrete particles. It would appear that the form to be expected for the spectral balance equation in the presence of both turbulence and sampling error is just Eq. (63), with $N^{(1)}$ reduced by a factor of W from the usual calculation of discreteness noise. This implies that all of the estimates given in Secs. V B 3 and V B 4 for the dependence of broadening and flux on discreteness level can be taken over intact, and would appear to justify the basic strategy adopted in Ref. 1. Of course, it is not sufficient to argue merely on the basis of a Kadomtsev-type equation (as I have done for pedagogical reasons), since that does not deal with wave-number-dependent quantities. The reader should consult Ref. 1 for the details of the more complete analyses and numerical experiments that support the conclusions of Nevins *et al.* that certain simulations can be noise-dominated.

VII. DISCUSSION AND CONCLUSIONS

A workhorse of modern plasma microturbulence theory is nonlinear gyrokinetics. The most physically transparent and numerically efficient form of that equation[20] displays the effects of ion polarization as a large "permittivity of the gyrokinetic vacuum"[4,22] and enables one to treat GK plasmas as Hamiltonian dynamical systems[21,72] in their own right. The Δf method proposes to solve the GKE by advancing in time the correction $\Delta f \doteq f - f_0$ from a given reference distribution. In general, f_0 is not the time-asymptotic steady-state distribution, in which case $\Delta f \neq \delta f$, where δf is the conventional fluctuation from the statistical mean.

The PIC approach to solving the Δf equation introduces Monte Carlo sampling error that can be treated quite similarly to the fluctuation noise associated with discrete particles in many-body plasmas. Sampling noise can mix with or indirectly affect the turbulent fluctuations, the simulation of which is the goal. Statistical formalism that systematically includes both turbulent signal and sampling noise can be developed. Although the details are extremely complicated in all generality, the structure of the theory is reasonably clear and sensible approximations can be made in the limit of small noise.

A source of some confusion in the literature has been the failure to clearly distinguish between (i) gyrokinetic plasmas consisting of discrete "particles" (gyrocenters); and (ii) the smooth Δf-Poisson system, one solution procedure for which is PIC. Although there are many similarities between the two models, their governing equations are not identical, and one's thinking can easily be led astray by failing to make the distinction.

The rigorous fluctuation-dissipation theorem applies only to discrete particle systems in thermal equilibrium. Because for weakly coupled systems the FDT can be formulated entirely in terms of the linear approximation to the dielectric function, it is easy to use; however, there is no justification (or necessity[132]) for using it away from thermal equilibrium, particularly for unstable plasmas. For slightly nonequilibrium but stable plasmas, the Klimontovich formalism leads to a fluctuation spectrum that is quite similar in form to the prediction of the FDT. It is the prediction of the nonequilibrium Klimontovich equation that naturally generalizes to steady turbulent states, not that of the FDT.

In turbulent states that are far from thermal equilibrium, the spectral balance equation replaces the FDT. Both have the general steady-state form

$$S(\boldsymbol{k},\omega) = \frac{N(\boldsymbol{k},\omega)}{|\mathcal{D}(\boldsymbol{k},\omega)|^2}. \tag{110}$$

The distinction is that in thermal equilibrium the numerator (forcing) function N is calculable from the imaginary part of the dielectric function $\mathcal{D}$, whereas that is not the case in general. Note that even in thermal equilibrium it is not trivial to calculate the fully nonlinear dielectric if the coupling is strong because $\mathcal{D}$ depends on the fluctuation level through all orders in the coupling. That problem is compounded in the nonequilibrium theory, in which two distinct functions (the response function R and the correlation function C) are coupled through all orders. A systematically renormalized theory appropriate for weak coupling is Rose's particle direct-interaction approximation (PDIA).[53]

The PDIA is a renormalization of the quadratically nonlinear Klimontovich equation. The statistical theory of sampling noise can be formulated as a renormalization problem for the coupled equations for Δf and the marker distribution $\tilde{N}_m$; however, that system is cubically nonlinear. Although Rose's methods could be generalized to handle such a system, no attempt has been made to do so here because of the considerable complexity of the general result. However, for weak coupling it was argued that one again recovers a balance equation of the form (110), in which the sampling noise is additive to the turbulent noise in the numerator N. The sampling noise spectrum is the one calculated from the discrete marker distribution, reduced by the mean-square particle weight.

Various discussions of the effects of sampling noise have been based on a heuristic spectral evolution equation proposed by Kadomtsev [Eq. (82)]. That equation is slightly too simplistic when discreteness noise is added because it fails to distinguish between the linear growth rate of collective instabilities and the damping rate of the discreteness noise (level I_0). However, it seems to capture the essence of the interplay between noise and mode coupling. The general form of the $\boldsymbol{k}$- and ω-dependent spectral balance equation can be used to derive Kadomtsev-type equations. One prediction from a simple piecewise-linear model of the dependence of spectral level on linear growth rate is that the total spectral broadening may decrease when I_0 is increased because the noise interferes with the linear excitation. If macroscopic transport coefficients are estimated from that broadening (which essentially amounts to equating the incremental and steady-state diffusion coefficients), then another prediction is that the total diffusion coefficient is reduced by increasing I_0, as argued in Ref. 1. These general arguments do not invoke the FDT.

Given that sensible estimates of the effects of sampling noise can be made, the reader may well ask, "Are Δf-PIC simulations noise-dominated or not?" The answer is clearly, "it depends." Modern simulations that are argued to be well converged are described, for example, in Refs. 3, 133, and 134, and many more will appear. However, that does not vitiate the need for workable analytical estimates of, and numerical diagnostics for, the effects of algorithmic noise along the lines described in Ref. 1.

In this article I have attempted to survey some of the theories of statistical dynamics as applied to both equilibrium and nonequilibrium situations. Although for nonlinear couplings of arbitrary size the theory is complex and defies simple quantitative predictions, qualitative arguments based on the general structure of the coupled renormalized equations for the correlation and response functions can be used to good advantage to make simple, testable predictions about the effects of sampling noise on transport and to motivate appropriate simulation diagnostics.[1] More generally, statistical methods are useful for many situations encountered in the physics of confined plasmas;[7] they deserve a place in the toolbox of every plasma theorist.

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APPENDIX A: FOURIER TRANSFORM CONVENTIONS

A consistent set of Fourier transform conventions is as follows. For discrete spatial transforms in a periodic box of length L, $A_k = L^{-1}\int_0^L dx\, e^{-ikx} A(x)$ and $A(x) = \Sigma_k e^{ikx} A_k$. For continuous transforms ($L \to \infty$), $A(k) = \int_{-\infty}^{\infty} dx\, e^{-ikx} A(x)$ and $A(x) = (2\pi)^{-1}\int_{-\infty}^{\infty} dk\, e^{ikx} A(k)$. One passes from a discrete representation to a continuous one by replacing $\Sigma_k \to \int_{-\infty}^{\infty} dk/\delta k$ ($\delta k \doteq 2\pi/L$ is the mode spacing) and $A_k \to A(k)/L$.

APPENDIX B: THE LOWEST-ORDER INFINITESIMAL RESPONSE FUNCTION

Here the form of the lowest-order infinitesimal response function is discussed in order to introduce the lowest-order dielectric function and to clarify the distinction between the response function R and the single-particle propagator g. In the absence of magnetic drifts, the gyrokinetic equation is

$$\partial_t F + v_\parallel \nabla_\parallel F + \bar{\boldsymbol{V}}_E \cdot \boldsymbol{\nabla} F + (q/m)\bar{E}_\parallel \partial_{v_\parallel} F = 0. \tag{B1}$$

If one introduces a generalized velocity $\boldsymbol{V} \doteq (\boldsymbol{V}_E, \hat{z} q E_\parallel / m)$ and a generalized derivative $\boldsymbol{\partial} \doteq (\boldsymbol{\nabla}_\perp, \hat{z}\partial_{v_\parallel})$, for future use adds a statistically sharp source of particles $\hat{\eta}$, and indicates random quantities by tildes, Eq. (B1) can be written as

$$\partial_t \tilde{F} + v_\parallel \nabla_\parallel \tilde{F} + \tilde{\bar{\boldsymbol{V}}} \cdot \boldsymbol{\partial} \tilde{F} = \hat{\eta}, \tag{B2}$$

where $\tilde{\bar{\boldsymbol{V}}} \doteq J_0 \tilde{\boldsymbol{V}}$ and $J_0 \equiv J_0(k_\perp v_\perp / \omega_c)$. By definition, the random infinitesimal response function $\tilde{R}$ is the Green's function that describes the response to an infinitesimal source, i.e., $\tilde{R}(z,t;z',t') \doteq \delta\tilde{F}(z,t)/\delta\hat{\eta}(z',t')$, where $\delta/\delta\hat{\eta}$ denotes functional differentiation. $\tilde{R}$ obeys

$$\partial_t \tilde{R} + v_\parallel \nabla_\parallel \tilde{R} + \tilde{\bar{\boldsymbol{V}}} \cdot \boldsymbol{\partial}\tilde{R} + \boldsymbol{\partial}\tilde{F} \cdot \hat{\bar{\boldsymbol{\mathcal{V}}}} \tilde{R} = \delta(z - z')\,\delta(t - t'), \tag{B3}$$

where $\hat{\boldsymbol{\mathcal{V}}}$ is the linear operator that converts distribution function to velocity: $\tilde{\boldsymbol{V}} = \hat{\boldsymbol{\mathcal{V}}}\tilde{F}$. The mean response function R is the statistical average of $\tilde{R}$, $R \doteq \langle \tilde{R} \rangle$. In general, the average of Eq. (B3) does not lead to a closed equation for R because Eq. (B3) is quadratic in random quantities. That problem is dealt with in the formal renormalization schemes.[58,7] However, if fluctuations are ignored, e.g., $\tilde{F} \approx \langle F \rangle$, then a solvable problem is defined for the lowest-order response function $R^{(0)}$:

$$(g^{(0)})^{-1} R^{(0)} + \boldsymbol{\partial}\langle F \rangle \cdot \hat{\bar{\boldsymbol{\mathcal{V}}}} R^{(0)} = \delta(z - z')\,\delta(t - t'), \tag{B4}$$

where the zeroth-order particle propagator $g^{(0)}$ has been introduced. $g^{(0)}$ is Green's function for zeroth-order particle motion:

$$(\partial_t + v_\parallel \nabla_\parallel + \langle \bar{\boldsymbol{V}} \rangle \cdot \boldsymbol{\partial}) g^{(0)} = \delta(z - z')\,\delta(t - t'). \tag{B5}$$

Subsequently I shall neglect any background velocity or electric field, $\langle \bar{\boldsymbol{V}} \rangle = \boldsymbol{0}$.

Equation (B4) is essentially the linearized gyrokinetic equation. It can be solved by simple operator manipulations. The formal solution of Eq. (B4) rewritten as $(g^{(0)})^{-1} R^{(0)} = \mathbf{I} - \boldsymbol{\partial}\langle F \rangle \cdot \hat{\bar{\boldsymbol{\mathcal{V}}}} R^{(0)}$ is

$$R^{(0)} = g^{(0)} - g^{(0)} \boldsymbol{\partial}\langle F \rangle \cdot \hat{\bar{\boldsymbol{\mathcal{V}}}} R^{(0)}. \tag{B6}$$

Upon applying $\hat{\bar{\boldsymbol{\mathcal{V}}}}$, one constructs an equation for the induced velocity:

$$\hat{\hat{\mathcal{V}}}R^{(0)} = \hat{\hat{\mathcal{V}}}g^{(0)} - \hat{\hat{\mathcal{V}}}g^{(0)}\boldsymbol{\partial}\langle F\rangle \cdot \hat{\hat{\mathcal{V}}}R^{(0)}, \tag{B7}$$

or, upon dividing out the J_0 implicit in $\hat{\hat{\mathcal{V}}}$,

$$(\mathbf{I} + \hat{\mathcal{V}}g^{(0)}J_0\boldsymbol{\partial}\langle F\rangle)\cdot\hat{\mathcal{V}}R^{(0)} = \hat{\mathcal{V}}g^{(0)}. \tag{B8}$$

The second-rank tensor on the left-hand side formally defines a dielectric tensor. However, in the electrostatic case where the velocity is a fixed (wave-number-dependent) vector times the electrostatic potential, it is not hard to show that the dielectric scalar

$$\mathcal{D}^{(0)} = 1 + \hat{\mathcal{V}}\cdot g^{(0)}J_0\boldsymbol{\partial}\langle F\rangle \tag{B9}$$

enters, and that

$$\hat{\mathcal{V}}R^{(0)} = (\mathcal{D}^{(0)})^{-1}\hat{\mathcal{V}}g^{(0)}. \tag{B10}$$

This solution can be inserted into Eq. (B6) to yield an expression for $R^{(0)}$ itself,

$$R^{(0)} = g^{(0)} - g^{(0)}J_0\boldsymbol{\partial}\langle F\rangle\cdot(\mathcal{D}^{(0)})^{-1}\hat{\mathcal{V}}g^{(0)}. \tag{B11}$$

Either of the forms (B6) and (B11) shows the important distinction between R and g, namely that R includes self-consistent response while g does not.

In the absence of magnetic drifts and for a Maxwellian background, one has

$$\hat{\mathcal{V}} = \left(\frac{c}{B}\hat{z}\times(i\boldsymbol{k}), -\frac{q}{m}ik_\parallel\right)\hat{\Phi}, \tag{B12a}$$

$$\boldsymbol{\partial} = (-L_n^{-1}\hat{\boldsymbol{x}}, -v_\parallel/v_t^2), \tag{B12b}$$

where $\hat{\Phi} \doteq 4\pi(\epsilon_{\mathrm{GV}}k^2)^{-1}\Sigma_s(\bar{n}q)_s\int d\boldsymbol{v}J_{0,s}$. One then obtains the lowest-order GK dielectric function in the form

$$\mathcal{D}_G^{(0)} = 1 + \sum_s\left(\frac{k_{Ds}^2}{\epsilon_{\mathrm{GV}}k^2}\right)\Gamma_s \times \int dv_\parallel\left(\frac{\omega_{*s} - k_\parallel v_\parallel}{\omega - k_\parallel v_\parallel + i\epsilon}\right)F_{M,s}(v_\parallel). \tag{B13}$$

In thermal equilibrium, ω_* must be set to zero; one then recovers Eq. (43).

A natural question is how to renormalize these lowest-order results. In the context of unmagnetized Vlasov theory, DuBois and Espedal[122] showed and Rose confirmed[53] that the form (B10) is preserved, i.e., $\hat{\mathcal{V}}R = \mathcal{D}^{-1}\hat{\mathcal{V}}g$, provided that $\mathcal{D}$ and g are renormalized appropriately (a subtle issue[7]). In fact, the form Eq. (B13) is preserved under renormalization provided a particular nonlinear correction is made to $\langle F\rangle$: $\langle F\rangle \to \bar{F} \doteq F + O(C)$.

APPENDIX C: GYROKINETIC NORMAL MODES

Let us consider the normal modes of the electrostatic gyrokinetic plasma, first in the absence of background gradients ($\omega_* = 0$). For Maxwellian background, one analyzes the roots of Eq. (B13),

$$0 = 1 + \sum_s\left(\frac{k_{Ds}^2}{\epsilon_{\mathrm{GV}}k^2}\right)\Gamma_s\int dv_\parallel\left(\frac{-k_\parallel v_\parallel}{\omega - k_\parallel v_\parallel + i\epsilon}\right)F_{M,s}(v_\parallel). \tag{C1}$$

It is easy to see that no normal modes exist for $\omega/k_\parallel \ll v_{ti}$, since in that limit the right-hand side of Eq. (C1) becomes positive-definite (both species respond adiabatically). In the intermediate regime $v_{ti} \ll \omega/k_\parallel \ll v_{te}$, the ion response is fluid-like and one may expand $(\omega - k_\parallel v_\parallel)^{-1} \approx \omega^{-1}(1 + k_\parallel v_\parallel/\omega)$. What results are the ion sound waves,

$$\omega^2 = \frac{k_\parallel^2\bar{c}_s^2}{1 + (k\lambda_{\mathrm{De}})^2\epsilon_{\mathrm{GV}}(\boldsymbol{k})}, \tag{C2}$$

where $\bar{c}_s^2 \doteq c_s^2\Gamma_i$. In the limit $T_i \to 0$,

$$1 + (k\lambda_{\mathrm{De}})^2\epsilon_{\mathrm{GV}}(\boldsymbol{k}) \approx 1 + k^2\lambda_{\mathrm{De}}^2 + k_\perp^2\rho_s^2 \approx 1 + k_\perp^2\rho_s^2, \tag{C3}$$

demonstrating the important shielding effect of the ion polarization drift. For $T_i = T_e$ (complete thermal equilibrium), these excitations are heavily damped and do not qualify as normal modes.

For $\omega/k_\parallel v_{te} \gg 1$, both species obey fluid response; one finds[20]

$$\omega^2 \approx \Omega_H^2 \doteq \left(\frac{k_\parallel^2}{k^2}\right)\frac{\bar{\omega}_p^2}{\epsilon_{\mathrm{GV}}(\boldsymbol{k})}. \tag{C4}$$

In this form, these high-frequency modes are seen to be essentially magnetized Langmuir oscillations, with response reduced by the plasma shielding. In the cold-ion, long-wavelength limit $\epsilon_{\mathrm{GV}} \approx \rho_s^2/\lambda_{\mathrm{De}}^2$, one finds that $\omega_p^2/\epsilon_{\mathrm{GV}} \approx |\omega_{ce}|\omega_{ci}$; thus these modes are variants of the lower hybrid waves. In the fluid limit, these modes are very weakly Landau damped and can be shown to carry virtually all of the equilibrium fluctuation energy. This is completely analogous to the situation in unmagnetized plasma, where the Langmuir waves carry the equilibrium energy when $k\lambda_{\mathrm{De}} \ll 1$.

For $\omega_* \neq 0$ and $v_{ti} \ll \omega/k_\parallel \ll v_{te}$, one finds the electron drift wave

$$\omega = \frac{\omega_{*e}\Gamma_i}{1 + (k\lambda_{\mathrm{De}})^2\epsilon_{\mathrm{GV}}(\boldsymbol{k})} \approx \frac{\omega_{*e}}{1 + k_\perp^2\rho_s^2}. \tag{C5}$$

Although the electrostatic approximation is useful for simple numerical tests and elucidation of basic physical processes, it is not necessarily realistic. Transition to an electromagnetic regime occurs nominally when the Alfvén velocity $c_A \doteq (B^2/4\pi n_i m_i)^{1/2}$ becomes smaller than the electron thermal velocity. One has $c_A^2/v_{te}^2 = \beta_e^{-1}(m_e/m_i)$, where $\beta_e \doteq 4\pi n_e T_e/B^2$; thus fluctuations are electromagnetic for $\beta_e > m_e/m_i$, which is easily satisfied. It can be shown[135] that when $k_\perp^2\delta_e^2 < 1$, where $\delta_e \doteq c/\omega_{pe}$ is the electron skin depth, the Ω_H modes metamorphose into shear Alfvén waves.[136] Although numerical algorithms appropriate for this regime, as well as the theory of fluctuations associated with the Alfvén waves,[135] are of considerable contemporary interest,[137] space constraints and my focus on spectral balance preclude a detailed discussion of electromagnetic effects here.

APPENDIX D: RECOVERY OF THE WEAKLY COUPLED FLUCTUATION SPECTRUM FROM THE DYSON EQUATIONS OF ROSE

In this appendix I sketch how to recover from Rose's Dyson equations the familiar spectrum (33) of weakly coupled discrete particles. Rose proved that

$$\langle \delta N(1,t)\delta N(2,t')\rangle_{+} = R(1,t;2,t')n_2^{-1}f(2,t') + C_{+}(1,t,2,t') + G_{3+}(1,t;2,t'_{+};2,t'), \tag{D1}$$

where the subscript + denotes a one-sided function in time. G_3 is a certain three-point cumulant. Rose explained that such cumulants can be expressed in terms of R, C, and a renormalized three-point vertex function Γ_3. Such vertex functions (generalized skewness) figured prominently in the original work of MSR; for some discussion, see Ref. 7. Rose also noted that in the PDIA one has $\Gamma_3 \approx \gamma_3$, where γ_3 is essentially the nonlinear coupling coefficient in the Klimontovich equation. I shall not write the explicit expression for G_3 here, but that function will be important momentarily.

We need the Fourier transform of the two-sided function $\langle \delta N(1)\delta N(2)\rangle$ (from which one can construct the field spectrum by applying $\hat{\boldsymbol{\mathcal{E}}}$ to both arguments), which is $2\,\mathrm{Re}\langle \delta N \delta N\rangle(\boldsymbol{k},\omega)$. Thus, omitting $(\boldsymbol{k},\omega)$ arguments,

$$\langle \delta \boldsymbol{E}\,\delta \boldsymbol{E}\rangle = 2\,\mathrm{Re}(\hat{\boldsymbol{\mathcal{E}}}Rn^{-1}f\hat{\boldsymbol{\mathcal{E}}}^{\dagger}) + \hat{\boldsymbol{\mathcal{E}}}C(\boldsymbol{k},\omega)\hat{\boldsymbol{\mathcal{E}}}^{\dagger} + \hat{\boldsymbol{\mathcal{E}}}G_3\hat{\boldsymbol{\mathcal{E}}}^{\dagger}. \tag{D2}$$

I have left C as the two-sided function because it is that function that is predicted from the Dyson equation: $C = R\Sigma_{--}R^{\dagger}$. One may use $\hat{\boldsymbol{\mathcal{E}}}R = \mathcal{D}^{-1}\hat{\boldsymbol{\mathcal{E}}}g$ to find

$$\langle \delta \boldsymbol{E}\,\delta \boldsymbol{E}\rangle = 2\,\mathrm{Re}(\mathcal{D}^{-1}\hat{\boldsymbol{\mathcal{E}}}gn^{-1}f\hat{\boldsymbol{\mathcal{E}}}^{\dagger}) + \frac{\hat{\boldsymbol{\mathcal{E}}}g\Sigma_{-}g^{\dagger}\hat{\boldsymbol{\mathcal{E}}}^{\dagger}}{|\mathcal{D}|^2} + \hat{\boldsymbol{\mathcal{E}}}G_3\hat{\boldsymbol{\mathcal{E}}}^{\dagger}. \tag{D3}$$

The first term can be written as

$$2\,\mathrm{Re}(\mathcal{D}^{-1}\hat{\boldsymbol{\mathcal{E}}}gn^{-1}f\hat{\boldsymbol{\mathcal{E}}}^{\dagger}) = \frac{2\,\mathrm{Re}[(1+\chi^{*})(\hat{\boldsymbol{\mathcal{E}}}gn^{-1}f\hat{\boldsymbol{\mathcal{E}}}^{\dagger})]}{|\mathcal{D}|^2}, \tag{D4}$$

where χ is the susceptibility. One can easily show that the first, vacuum, term reduces precisely to the desired result if one uses the zeroth-order propagator $g^{(0)}$. Thus,

$$2\,\mathrm{Re}(\hat{\boldsymbol{\mathcal{E}}}g^{(0)}n^{-1}f\hat{\boldsymbol{\mathcal{E}}}^{\dagger}) = 2\epsilon_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}^{*}\mathrm{Re}\sum_{s,s'}(\bar{n}q)_s(\bar{n}q)_{s'}\int d\boldsymbol{v}\,d\boldsymbol{v}' \times \frac{\delta(\boldsymbol{v}-\boldsymbol{v}')\delta_{s,s'}}{-i(\omega-\boldsymbol{k}\cdot\boldsymbol{v}+i\epsilon)}\frac{1}{n_{s'}}f_{s'}(\boldsymbol{v}') \tag{D5a}$$

$$= 2\pi\epsilon_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}^{*}\sum_{s}(\bar{n}q^2)_s\int d\boldsymbol{v}\,\delta(\omega-\boldsymbol{k}\cdot\boldsymbol{v})f_s(\boldsymbol{v}). \tag{D5b}$$

By using Rose's approximate form (88) of Σ_{--} and the result $G_3 \approx RRC\gamma_3$, one can also show with straightforward algebra that the χ term is canceled by $\Sigma_{--}^{(1)}$.

By recovering the usual fluctuation spectrum from the renormalized field theory, I have demonstrated a necessary consistency. The exercise emphasizes that the distinction between $\langle \delta N \delta N\rangle$ and C (well known in Klimontovich theory) must be handled with care. It also provides insight that will be of use when we consider the second-order theory, as will be seen in Sec. V B 3.

[1] W. M. Nevins, G. W. Hammett, A. M. Dimits, W. Dorland, and D. E. Shumaker, Phys. Plasmas **12**, 122305 (2005).
[2] A. M. Dimits, G. Bateman, M. A. Beer, B. I. Cohen, W. Dorland, G. W. Hammett, C. Kim, J. E. Kinsey, M. Kotschenreuther, A. H. Kritz *et al.*, Phys. Plasmas **7**, 969 (2000).
[3] W. M. Nevins, J. Candy, S. Cowley, T. Dannert, A. Dimits, W. Dorland, C. Estrada-Mila, G. W. Hammett, F. Jenko, M. J. Pueschel, and D. E. Shumaker, Phys. Plasmas **13**, 122306 (2006).
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[13] L. D. Landau, Phys. Z. Sowjetunion **10**, 154 (1936) [Zh. Eksp. Teor. Fiz. **7**, 203 (1937)].
[14] Y. L. Klimontovich, *The Statistical Theory of Nonequilibrium Processes in a Plasma*, edited by D. ter Harr, translated by H. S. H. Massey and O. M. Blunn (MIT, Cambridge, MA, 1967).
[15] C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation* (McGraw-Hill, New York, 1985).
[16] A. B. Langdon and C. K. Birdsall, Phys. Fluids **13**, 2115 (1970).
[17] R. L. Morse and C. W. Nielson, Phys. Fluids **12**, 2418 (1969).
[18] A. B. Langdon, Phys. Fluids **22**, 163 (1979).
[19] E. A. Frieman and L. Chen, Phys. Fluids **25**, 502 (1982).
[20] W. W. Lee, Phys. Fluids **26**, 556 (1983).
[21] D. H. E. Dubin, J. A. Krommes, C. R. Oberman, and W. W. Lee, Phys. Fluids **26**, 3524 (1983).
[22] J. A. Krommes, W. W. Lee, and C. Oberman, Phys. Fluids **29**, 2421 (1986).
[23] J. A. Krommes, Phys. Rev. Lett. **70**, 3067 (1993).
[24] M. Kotschenreuther, in *Proceedings of the 14th International Conference on the Numerical Simulation of Plasmas* (Office of Naval Research, Arlington, Virginia, 1991), paper PT20.
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[26] A. M. Dimits and W. W. Lee, J. Comput. Phys. **107**, 309 (1993).
[27] S. E. Parker and W. W. Lee, Phys. Fluids B **5**, 77 (1993).
[28] A. Y. Aydemir, Phys. Plasmas **1**, 822 (1994).
[29] I am well aware that it is conventional in the simulation literature to use δf rather than Δf for the correction to the reference distribution. Unfortunately, that usage conflicts with a long-established convention for fluctuations about the mean, $f = \langle f\rangle + \delta f$, where the angle brackets denote an ensemble average. In general, $\Delta f \neq \delta f$. This is explained in detailed in Sec. II B.
[30] Aydemir (Ref. 28) discussed how the Δf algorithm is related to the control-variate technique of basic Monte Carlo theory.
[31] Because the rigorous equation for $\dot{w}$ involves a factor of $1-w$ in the driving term [Eq. (58)], the weights cannot grow beyond $w=1$. That, however, is outside the region of validity of the Δf approach.
[32] W. W. Lee and W. M. Tang, Phys. Fluids **31**, 612 (1988).
[33] J. A. Krommes and G. Hu, Phys. Plasmas **1**, 3211 (1994).
[34] In detail, the dissipation mechanism in the work of Watanabe and Sugama (Ref. 35) was physical collisions, whereas the dissipation invoked by

Candy and Waltz (Ref. 36) arose from the numerical scheme. The arguments of Krommes and Hu (Ref. 33) suggest that in some circumstances the origin of the dissipation may not matter.

[35] T.-H. Watanabe and H. Sugama, Phys. Plasmas **11**, 1476 (2004).

[36] J. Candy and R. E. Waltz, Phys. Plasmas **13**, 032310 (2006).

[37] A preliminary suggestion for dealing with this problem was given in Ref. 39.

[38] The scenario discussed by Nevins *et al.* (Ref. 1) involved the noise suppressing the turbulence rather than the noise growing up to overwhelm a fixed-amplitude signal.

[39] J. A. Krommes, Phys. Plasmas **6**, 1477 (1999).

[40] S. Brunner, E. Valeo, and J. A. Krommes, Phys. Plasmas **6**, 4504 (1999).

[41] S. Vadlamani, S. E. Parker, Y. Chang, and C. Kim, Comput. Phys. Commun. **164**, 209 (2004).

[42] Y. Chen and S. E. Parker, Phys. Plasmas **14**, 082301 (2007).

[43] Note that I distinguish various disparate quantities solely by their arguments; the symbols $C_{\boldsymbol{k}}(t)$, $C_{\boldsymbol{k}}(\tau)$, and $C_{\boldsymbol{k}}(\omega)$ denote three independent functions.

[44] R. H. Kraichnan, Phys. Fluids **7**, 1163 (1964).

[45] In discussions of Navier-Stokes turbulence, dielectric functions are not usually mentioned, although they should be. J. A. Krommes and P. L. Similon [Phys. Fluids **23**, 1553 (1980)] discussed the special case of the guiding-center plasma, which shows very clearly how R is related to $\mathcal{D}^{-1}$ in a fluid-like model. In kinetic problems with a velocity variable, R most fundamentally describes the kinetic response, while $\mathcal{D}^{-1}$ emerges after integration of R over velocity; the key result is the shielding relation (89).

[46] N. A. Krall and A. W. Trivelpiece, *Principles of Plasma Physics* (McGraw-Hill, New York, 1973).

[47] T. G. Jenkins and W. W. Lee, Phys. Plasmas **14**, 032307 (2007).

[48] For quadratically nonlinear dynamics, spatial homogeneity dictates that the triangle relation $\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q}=\boldsymbol{0}$ must always be satisfied. ω' and ω'' need not refer to normal modes $\Omega_{\boldsymbol{p}}$ and $\Omega_{\boldsymbol{q}}$. The normal-mode frequency-matching condition $\Omega_{\boldsymbol{k}}+\Omega_{\boldsymbol{p}}+\Omega_{\boldsymbol{q}}=0$ is required in weak turbulence theory, but not in general.

[49] Due to homogeneity, $R^{(n)}$ depends on $n-1$ spatial coordinates; my convention is to refer them to $\boldsymbol{x}$, viz., $R^{(2)}(\boldsymbol{x};\boldsymbol{x}',\boldsymbol{x}'')=R^{(2)}(\boldsymbol{x}-\boldsymbol{x}',\boldsymbol{x}-\boldsymbol{x}'')$, then to Fourier transform with respect to the difference coordinates.

[50] One might argue that one can always initialize the system in such as way that $\mathrm{Re}\,\eta_{\boldsymbol{k}}^{\mathrm{nl}} \ll \gamma_{\boldsymbol{k}}$. However, such states are not stationary and must evolve until the inequality is reversed (assuming that the model is complete enough to guarantee a steady state).

[51] Equation (6) can be derived directly by integrating Eq. (1) over ω with the assumption $F_{\boldsymbol{k}}(\omega)=2F_{\boldsymbol{k}}$. The discussion in this section is intended to be pedagogical, not overly technical. A much more thorough and systematic derivation of the equal-time balance equation was given by G. F. Carnevale and P. C. Martin [Geophys. Astrophys. Fluid Dyn. **20**, 131 (1982)]. Some aspects of that paper were discussed by J. Krommes and C.-B. Kim [Phys. Rev. E **62**, 8508 (2000)]; see also Appendices F and G of Ref. 7.

[52] S. A. Orszag, in *Fluid Dynamics*, edited by R. Balian and J.-L. Peube (Gordon and Breach, New York, 1977), pp. 235–374.

[53] H. A. Rose, J. Stat. Phys. **20**, 415 (1979).

[54] B. B. Kadomtsev, *Plasma Turbulence* (Academic, New York, 1965), translated by L. C. Ronson from the 1964 Russian edition, *Problems in Plasma Theory*, edited by M. A. Leontovich, translation edited by M. C. Rusbridge.

[55] μ is conserved in gyrokinetics, so no derivative with respect to μ appears.

[56] J. A. Krommes and C.-B. Kim, Phys. Fluids **31**, 869 (1988).

[57] In a strict interpretation, f cannot be random because it is already a PDF; specifically, it is the ensemble average of the Klimontovich microdensity. Frequently, however, multiple-scale averaging is used wherein only averages over sub-Debye scales are imagined to be performed explicitly, removing particle discreteness in favor of the plasma collision operator. That is ignored in the collisionless approximation and one is left with a stochastic equation with averages over super-Debye scales remaining to be performed.

[58] P. C. Martin, E. D. Siggia, and H. A. Rose, Phys. Rev. A **8**, 423 (1973).

[59] The dissertation by Jenkins (Ref. 81) describes a more complete formalism containing two distinct weights (first introduced in Ref. 5). It can also serve as a useful introduction to GK PIC techniques.

[60] L. D. Landau and E. M. Lifshitz, *Statistical Physics, Part I*, 3rd ed. (Pergamon, Oxford, 1980), revised and enlarged by E. M. Lifshitz and L. P. Pitaevskii, translated from the Russian by J. B. Sykes and M. J. Kearsley, Chap. XII.

[61] The correction term V^{-1} (frequently omitted) ensures that the $\boldsymbol{k}=\boldsymbol{0}$ Fourier component of $C(\boldsymbol{x}-\boldsymbol{x}')$ vanishes.

[62] P. C. Martin, in *Many Body Physics*, edited by C. deWitt and R. Balian (Gordon and Breach, New York, 1968), pp. 37–136.

[63] G. Ecker, *Theory of Fully Ionized Plasmas* (Academic, New York, 1972), Chap. I.

[64] When electromagnetic effects are important, one must introduce a dielectric tensor; see Ref. 4.

[65] Strictly speaking, this result is valid only for the Vlasov dielectric $\mathcal{D}^{(0)}$. When higher-order terms in ϵ_p are included, the Debye length is slightly modified [see F. Tappert, Ph.D. thesis, Princeton University (1967)]. There are also corrections for scales of the order of the distance of closest approach.

[66] One must take due account of modifications due to the use of finite-size particles and numerical smoothing; see Ref. 15 for details and references.

[67] Ion sound waves are heavily Landau damped in thermal equilibrium ($T_e=T_i$) so do not qualify as normal modes.

[68] In fact, the integral for C_{EE} is divergent as $|k|\to\infty$. That can be cured by asymptotically matching to a more complete formula at small scales. In simulations, the structure factor defining the finite-sized particles provides a natural cutoff (Ref. 16). Also, the integral for $\langle\delta\phi^2\rangle$ is convergent.

[69] In the products $\widetilde{N}\widetilde{N}\sim\Sigma_i\Sigma_j$ that occur, the self-interactions $j=i$ must be excluded.

[70] J. A. Krommes, Phys. Fluids **19**, 649 (1976).

[71] N. Rostoker, Phys. Fluids **7**, 479 (1964); **7**, 491 (1964).

[72] A. J. Brizard and T. S. Hahm, Rev. Mod. Phys. **79**, 421 (2007).

[73] J. A. Krommes, in *Turbulence and Coherent Structures in Fluids, Plasmas and Nonlinear Media*, edited by M. Shats and H. Punzmann (World Scientific, Singapore, 2006), pp. 115–232.

[74] T. H. Stix, *Waves in Plasmas* (AIP, New York, 1992).

[75] There is some confusion in the literature as to exactly what "the" gyrokinetic equation is. Frieman and Chen (Ref. 19) refer to the equation for a quantity h that is "essentially" the nonadiabatic portion of the gyrocenter PDF F, whereas I consider the equation for F itself. The two equations are physically equivalent. The disadvantages of the Frieman-Chen form are (i) it is not in characteristic form, (ii) the time derivative of the effective potential appears on the right-hand side of the h equation, and (iii) the important polarization drift is obscured.

[76] There should be no confusion between the uses of F for both the gyrocenter distribution function and the covariance of nonlinear random forcing [see, e.g., Eq. (1)].

[77] Thus polarization drift is not a "finite-Larmor-radius correction."

[78] Distinguish the sound radius ρ_{s} (Roman subscript) from the species-dependent gyroradius ρ_s.

[79] Another useful relation is that $\omega_{pi}^2/\omega_{ci}^2=c^2/c_A^2$, where $c_A \doteq (B^2/4\pi n_i m_i)^{1/2}$ is the Alfvén velocity.

[80] If one looks casually at the second term of Eq. (45a), one may perhaps be tempted to conclude that it is relatively large because of the ϵ_{GV} in the numerator, so C_{EE}^G would appear to be negative. That is not the case because ϵ_{GV} is large only for $k\rho_{\mathrm{s}}=O(1)$, in which case the denominator is also large. For $k\to\infty$, $\epsilon_{\mathrm{GV}}\to 1$.

[81] T. G. Jenkins, Ph.D. thesis, Princeton University (2007).

[82] G. W. Hammett (private communication, 2007).

[83] This approximation does not apply to convective-cell fluctuations with $k_\parallel=0$.

[84] Similar constructions and manipulations arise in the theory of laser scattering; see, for example, Ref. 46, Chap. 11.

[85] M. Kotschenreuther, G. Rewoldt, and W. M. Tang, Comput. Phys. Commun. **88**, 128 (1995); W. Dorland, F. Jenko, M. Kotschenreuther, and B. N. Rogers, Phys. Rev. Lett. **85**, 5579 (2000).

[86] F. Jenko, Comput. Phys. Commun. **125**, 196 (2000).

[87] J. Candy and R. Waltz, J. Comput. Phys. **186**, 545 (2003).

[88] I am grateful to G. Hammett (private communication, 2007) for emphasizing this point.

[89] M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods* (Wiley, New York, 1986), Vol. I.

[90] This is the basic insight underlying the seminal work of Ref. 16, which showed how the use of finite-sized particles coarse-grains the Klimontovich equation into the Vlasov equation.

[91] Compressible flows can be treated as well; see Ref. 5.

[92] In practice, the $p=1-w$ term on the right-hand side of Eq. (58) is frequently approximated by 1; most particle weights never become very large for the microturbulence of interest. Particles in the tail of the distribution

($F_m \to 0$) can cause problems; those are monitored and dealt with separately (W. W. Lee, private communication, 2007).

[93] Here and elsewhere in the article linear instability appears to be significant [J. A. Krommes, Plasma Phys. Controlled Fusion **41**, A641 (1999)]. The discussion must be appropriately modified if nonlinear instability (submarginal turbulence) is important. The common feature is that both linear and nonlinear instability are driven by the same sources of free energy (e.g., profile gradients). Note that there always exists a drive level below which even nonlinear instability is suppressed, although that may not coincide with the threshold for linear instability.

[94] This remark embraces the possibility of nonlinear instability (submarginal turbulence).

[95] D. Ruelle and F. Takens, Commun. Math. Phys. **20**, 167 (1971).
[96] A. J. Lichtenberg and M. A. Lieberman, *Regular and Chaotic Dynamics*, 2nd ed. (Springer, New York, 1992).
[97] W. D. McComb, *The Physics of Fluid Turbulence* (Clarendon, Oxford, 1990).
[98] M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. **17**, 323 (1945); reprinted in *Selected Papers on Noise and Stochastic Processes*, edited by N. Wax (Dover, New York, 1954), p. 113.

[99] The Gaussian assumption can be made more precise by considering a coarse-graining of the time axis into units of time much larger than the microscopic autocorrelation time, then invoking the central limit theorem.

[100] If $\langle\psi\rangle \neq 0$, it can be taken into account by modifying the linear operator $\hat{L}$.

[101] F. J. Dyson, Phys. Rev. **75**, 486 (1949).
[102] R. H. Kraichnan, J. Fluid Mech. **5**, 497 (1959).
[103] C. E. Leith, J. Atmos. Sci. **28**, 145 (1971).
[104] R. H. Kraichnan, J. Fluid Mech. **41**, 189 (1970).

[105] The DIA possesses another important amplitude representation, the random coupling model (Refs. 115 and 138), that was in fact discovered much earlier than the Langevin model.

[106] R. H. Kraichnan, in *Nonlinear Dynamics*, edited by R. H. G. Helleman (New York Academy of Sciences, New York, 1980), p. 37.
[107] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).
[108] J. C. Bowman, J. A. Krommes, and M. Ottaviani, Phys. Fluids B **5**, 3558 (1993).

[109] I have included factors of 2 for notational consistency.

[110] It is not guaranteed that steady states exist for arbitrary L_k. If they do not, the physical model is inadequate and must be refined.

[111] G. F. Carnevale, U. Frisch, and R. Salmon, J. Phys. A **14**, 1701 (1981).
[112] T. Carleman, Acta Vet. Acad. Sci. Hung. **174**, 1680 (1922).
[113] R. Kubo, J. Phys. Soc. Jpn. **17**, 1100 (1962).

[114] The combinatoric factors all reduce to 1 if one considers expansions of moments of distinct random variables.

[115] R. H. Kraichnan, J. Math. Phys. **2**, 124 (1961); **3**, 205(E) (1962).
[116] J. C. Bowman, Ph.D. thesis, Princeton University (1992).
[117] G. Hu, J. A. Krommes, and J. C. Bowman, Phys. Lett. A **202**, 117 (1995).
[118] G. Hu, J. A. Krommes, and J. C. Bowman, Phys. Plasmas **4**, 2116 (1997).
[119] J. C. Bowman and J. A. Krommes, Phys. Plasmas **4**, 3895 (1997).
[120] H. A. Rose, Ph.D. thesis, Harvard University (1974).
[121] M. Doi, J. Phys. A **9**, 1465 (1976).
[122] D. F. DuBois and M. Espedal, Plasma Phys. **20**, 1209 (1978).
[123] J. A. Krommes, in *Theoretical and Computational Plasma Physics* (International Atomic Energy Agency, Vienna, 1978), pp. 405–417.

[124] Because $H(0)=1/2$, $\langle\delta N(1,t)\delta N(2,t)\rangle_+ = 1/2\overline{n}_2^{-1}\delta(1-2)F(2,t) + C_+(1,t,2,t)$. Equation (85b) is recovered by noting that $\langle\delta N(t)\delta N(t)\rangle = \langle\delta N(t)\delta N(t)\rangle_+ + \langle\delta N(t)\delta N(t)\rangle_-$.

[125] M. Kruskal, in *Plasma Physics* (International Atomic Energy Agency, Vienna, 1965), p. 373.
[126] R. B. White, *Asymptotic Analysis of Differential equations* (Imperial College, London, 2005).
[127] A. Rogister and C. Oberman, J. Plasma Phys. **2**, 33 (1968); **3**, 119 (1969).

[128] See, for example, formula (16) of Ref. 1.

[129] W. W. Lee, Bull. Am. Phys. Soc. **51**, 111 (2006).
[130] T. H. Dupree, Phys. Fluids **9**, 1773 (1966).
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