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ABSTRACT

Monte-Carlo operators for the orbit-averaged Fokker-Planck equation describing collisions and wave-particle interaction are constructed. Special emphasis is put on ion-cyclotron-resonance heating of tokamaks, but the results are applicable to general quasilinear processes in arbitrary magnetic configurations in which particle motion is integrable. All effects of non-standard orbit topology, such as large orbit widths are fully taken into account. The Monte-Carlo operators may be used for simulating, e.g., neoclassical transport, radio-frequency heating, and wave-driven spatial diffusion.

I. INTRODUCTION

Fast ions, i.e. ions with energies much above the thermal, play a prominent role in the heating of fusion plasmas. In present-day tokamaks, minority ions accelerated by ion-cyclotron-resonance heating (ICRH) frequently reach energies in the MeV range[1,2], and deliver tens of megawatts of heating power to the bulk plasma. In a future reactor, most of the heating will be provided by fusion-generated alpha-particles. Apart from providing the heating power needed to sustain the plasma, the presence of fast ions can, because of their high energy content, also significantly affect the magnetohydrodynamic stability of the plasma. For instance, fishbone oscillations[3,4] and monster sawteeth[5] are believed to be caused by fast ions. In these respects, ICRH accelerated ions play a role similar to that of alpha-particles, and much insight into the behavior of alpha-particles can be gained by studying ICRH.

From the above it is clear that it is important to have a proper modelling of fast ions accelerated by ICRH. In particular, the modelling should be accurate enough to enable a detailed comparison with experimental results. One of the complications arising in the description of fast ions in tokamaks is that the radial width of the orbits tends to be very large, so that the usual small-banana-width approximation is invalid[6,7]. In the first part of this paper, we derive an orbit-averaged Fokker-Planck equation which describes the effects of collisions and resonant wave-particle interaction, with special emphasis on ICRH. The equation is valid in an arbitrary axisymmetric geometry and takes all effects associated with the finite width of drift orbits into account. One way of (numerically) solving the Fokker-Planck equation is to use Monte-Carlo techniques[8]. The required Monte-Carlo operators are derived in the latter part of the paper. These operators can, of

course, also be used to study problems involving particle sources, such as neutral-beam injection and production of fast ions in fusion reactions.

The distribution function in an orbit-averaged Fokker-Planck equation is a function of the invariants describing single particle motion. In the zero-banana-width approximation, the equation is two-dimensional in velocity space, with, e.g., the velocity and the magnetic moment as invariants of the motion. A number of codes solving this 2D equation have been developed[9,10,11]. When the radial width of the orbits is taken into account, the equation becomes three-dimensional, and three invariants are required. In order to keep our results as general and widely useful as possible, we do not restrict the discussion to any particular set of invariants, but formulate the kinetic equation and Monte-Carlo operators in terms of invariants of a fairly general form. The 3D character of the equation reflects that diffusion and convection take place both in velocity space and in real space. Neoclassical effects enter through the collision operator, and the RF-operator introduces additional radial convection and diffusion.

Simplified versions of the orbit-averaged Fokker-Planck equation have been used previously to study the slowing-down of alpha particles[12], but only collisional drag was taken into account. Furthermore, the influence of RF-induced diffusion has also been investigated[13,14,15], but without accounting for finite orbit width. Recently, Zaitsev, O'Brien and Cox[16] derived an orbit-averaged kinetic equation, in a form similar to ours, describing collisions but not wave-particle interaction.

Monte-Carlo techniques are very powerful for solving multidimensional diffusion problems, and orbit-following Monte-Carlo codes for studying fast ions produced by neutral-beam injection or ICRH have been constructed previously[7,17]. These codes follow drift orbits and apply Monte-Carlo operators a number of times each turn around the orbit. This method is slightly inefficient, since similar orbits have to be calculated over and over again. A faster way is to solve the orbit-averaged Fokker-Planck equation directly with a Monte-Carlo technique[18]. Such an approach has been used recently in a code developed to study the influence of stochastic ripple diffusion[19] (in the zero-banana-width limit). In this paper, we also follow this approach. There are several advantages with the Monte-Carlo technique: the central part of the computer program is not very complicated, and there are no particular problems with boundary conditions.

The paper is organized as follows: The averaging of the Fokker-Planck equation is carried out in Sec. II . For this, we find it very convenient to employ the Hamiltonian action-angle variables introduced by Kaufman[20], although we do not restrict the subsequent results to the use of these variables. In Sec. III, the averaged collisional and quasilinear operators are presented. Sec. IV contains the derivation of 3D Monte-Carlo operators from the kinetic equation, and, finally, our conclusions are summarized in Sec. V.

II. THE ORBIT-AVERAGED KINETIC EQUATION

In general, the kinetic equation describing the distribution function of a particle species interacting with a (weak) wave field has the form

$$\frac{\partial f}{\partial t} + \dot{z}^i \frac{\partial f}{\partial t} = C(f) + Q(f) \tag{1}$$

where C(f) is the collision operator, Q(f) is the quasilinear wave-particle interaction operator, and z^i are arbitrary phase-space coordinates. For instance, we may choose $z^i=(\mathbf{v},\mathbf{q})$, where $\mathbf{q}$ denotes the usual Cartesian coordinates and $\dot{\mathbf{q}} = \mathbf{v}$ Summation over repeated indices is understood throughout this paper.

In hot tokamak plasmas, the characteristic time-scales on which C(f) and Q(f) operate are generally large in comparison with the time it takes for a particle to complete an orbit (hereafter called the bounce time, τ_b). Instead of dealing with the equation (1) directly, it is then advantageous to take the orbit average of it. The most elegant way of doing this is to use action-angle variables. Since the motion of a single particle in an axisymmetric torus is integrable, it is possible to show[20,21] that there exist action-angle variables $(\mathbf{J},\boldsymbol{\theta})$, such that the (unperturbed) Hamiltonian H_0 depends only on the action variables, $H_0=H_0(\mathbf{J})$, and the angles evolve linearly in time:

$$\dot{\theta}^i = \frac{\partial H_0}{\partial J^i} = \Omega^i(\mathbf{J}) \tag{2}$$

Here, Ω^1 is the orbit-averaged cyclotron frequency, $\Omega^2=2\pi/\tau_b=\omega_b$ is the bounce frequency, and $\Omega^3 = <\dot{\varphi}>$ is the orbit-averaged time derivative of φ, the toroidal angle[20]. Roughly speaking, the first angle θ^1 describes the position of the particle

in the Larmor rotation, θ^2 the position along the guiding-center orbit, and θ^3 the toroidal position of the banana center. The action variables J^1 and J^3 are

$$\begin{aligned} J^1 &= m\mu / Ze = m^2 v_\perp^2 / 2ZeB \\ J^3 &= p_\varphi = mb_\varphi R v_\parallel + Ze\psi_p / 2\pi \end{aligned} \tag{3}$$

where m is the mass, Ze is the charge, R is the major radius coordinate, B is the magnetic field strength, $b_\varphi = R\nabla\varphi \cdot \mathbf{B} / B$, and ψ_p is the poloidal magnetic flux. (The poloidal magnetic field is taken to be $\mathbf{B}_p = \nabla\psi_p \times \nabla\varphi / 2\pi$..) The expression for the (canonical) toroidal angular momentum, p_φ, given here pertains to the guiding center. It is equal to that of the particle to all orders in a gyroradius expansion[22]. For brevity, we have not given the explicit expression for J^2; in fact we shall not need it. For a more detailed exposition of the action-angle variables, we refer the reader to Ref. [20].

The orbit average is defined simply as the integral over $\boldsymbol{\theta}$-space:

$$<\cdots> = (2\pi)^{-3} \iiint (\cdots) d\theta_1 d\theta_2 d\theta_3 \tag{4}$$

Because of axisymmetry and the fact that the gyroradius is usually small, the integrations over θ_1 and θ_3 are trivial, and (4) simply amount to

$$<\cdots> = (2\pi)^{-1} \int_0^{2\pi} (\cdots) d\theta_2 \tag{5}$$

The action-angle variables are convenient for averaging the kinetic equation (1) over orbits, but because the expression for J^2 is complicated (It involves an integral over the orbit.), we do not wish to write the resulting equation in these variables, but in some other, arbitrary, set of invariants $\mathbf{I}=\mathbf{I}(\mathbf{J})$. In addition, we want to keep the formalism as flexible as possible. In the coordinates $x^i = (\mathbf{I},\boldsymbol{\theta})$, the kinetic equation (1) reads

$$\frac{\partial f}{\partial t} + \Omega^i(\mathbf{I}) \frac{\partial f}{\partial t} = C(f) + Q(f) \tag{6}$$

and after averaging, we have

$$\frac{\partial f_0}{\partial t} = < C(f_0) + Q(f_0) > \tag{7}$$

where $f_0 = \langle f \rangle$. We now turn to the right-hand side of this equation, where we have approximated f by f_0. The collision operator conserves particles in each point of coordinate space, and can, consequently, be written as a divergence, $C(f)=\partial C^i/\partial v^i=$
$\partial C^i/\partial z^i$. Transforming to the variables $x^i = (\mathbf{I},\boldsymbol{\theta})$, we have

$$C(f) = g^{-1/2}\frac{\partial}{\partial x^i}(g^{1/2}\,\Gamma^i) \tag{8}$$

where Γ^i are the contravariantly transformed components of C^i, $\Gamma^i=C^j\partial x^i/\partial z^j$, and $g^{1/2}$ is the Jacobian $g^{1/2} = |\partial \mathbf{z}/\partial \mathbf{x}|$. The latter is independent of the angles θ, since

$$g^{1/2} = \left|\frac{\partial(\mathbf{v},\mathbf{q})}{\partial(\mathbf{I},\theta)}\right| = m^{-3}\left|\frac{\partial(\mathbf{J},\theta)}{\partial(\mathbf{I},\theta)}\right| = m^{-3}\left|\frac{\partial \mathbf{J}}{\partial \mathbf{I}}\right| \tag{9}$$

and the averaging of the collision operator is therefore very simple:

$$\langle C(f)\rangle = g^{-1/2}\frac{\partial}{\partial \mathbf{I}^i}\left(g^{1/2}\langle \Gamma^i \rangle\right) \tag{10}$$

The quasilinear operator Q(f) has been derived by Kaufman[20], and has the following simple form when expressed in action variables

$$Q(f) = \frac{\partial}{\partial J^i}\left(\overline{D}^{ij}\frac{\partial f}{\partial J^j}\right) \tag{11}$$

Note that this operator does not depend on the angles, and need therefore not be averaged in (7). Transforming to the variables **I**, we obtain

$$\begin{aligned} Q(f) &= g^{-1/2}\frac{\partial}{\partial I^i}\left(g^{1/2}D^{ij}\frac{\partial f}{\partial I^j}\right) \\ D^{ij} &= \frac{\partial I^i}{\partial J^k}\frac{\partial I^j}{\partial J^l}\overline{D}^{kl} \end{aligned} \tag{12}$$

where the derivatives $\partial I^i/\partial J^k$ can easily be calculated by using Eqs (2) and (3). (For a specific example of this, see Sec. IV B.) The formal derivation of the orbit averaged kinetic equation is now complete; the result is expressed in Eqs (7), (9), (10) and (12). In the next section, we shall give more explicit expressions for the collisional and quasilinear operators.

III. THE COLLISIONAL AND QUASILINEAR OPERATORS

The collision operator is, of course, very well known. When averaged over Larmor rotation and written in the velocity coordinates (v,χ) where $\chi = v_{\|} / v$, it has the form[23,24]

$$C(f) = \frac{1}{v^2}\frac{\partial}{\partial v}\left[v^2\left(A^v f + T^{vv}\frac{\partial f}{\partial v} + T^{v\chi}\frac{\partial f}{\partial \chi}\right)\right] + \frac{\partial}{\partial \chi}\left(A^\chi f + T^{\chi v}\frac{\partial f}{\partial v} + T^{\chi\chi}\frac{\partial f}{\partial \chi}\right) \quad (13)$$

where the components of A and T are given in the Appendix.

We now turn to the quasilinear operator. In the presence of a wave field, the Hamiltonian of the system is perturbed, $H=H_0+H_1$, where

$$H_1 = -Ze\,\mathbf{A}\cdot\mathbf{v} + Ze\Phi = \left\{ \mathbf{E} = \sum_\omega \mathbf{E}_\omega e^{-i\omega t}\right\} = -\sum_\omega \frac{iZe}{\omega}\,\mathbf{v}\cdot\mathbf{E}_\omega \quad (14)$$

Here $\mathbf{A}$ and Φ are the magnetic and electrostatic potentials of the wave field $\mathbf{E}$. Kaufman's expression for the diffusion tensor $\bar{D}^{ij}$ in Eq.(12) is[20]

$$\overline{D}^{ij} = \pi \sum_{\mathbf{n},\omega} \left| H_1(\mathbf{J},\mathbf{n},\omega)\right|^2 \delta(\omega - \mathbf{n}\cdot\Omega) n^i n^j \quad (15)$$

where $\mathbf{n}=(n^1,n^2,n^3)$ is a vector of integers, and $H_1(\mathbf{J},\mathbf{n},\omega)$ is the Fourier transform of H_1 with respect to the angles $\boldsymbol{\theta}$ and the time t :

$$H_1(\mathbf{J},\boldsymbol{\theta},t) = \sum_{\mathbf{n},\omega} H_1(\mathbf{J},\mathbf{n},\omega)\, e^{i(\mathbf{n}\cdot\boldsymbol{\theta}-\omega t)} \quad (16)$$

The integer n^3 is always equal to the toroidal wave number N, and in the case of ICRH at the n:th harmonic of the cyclotron frequency, $n^1=n$. Standard manipulations of (14) and (16) then give[25,26]

$$\begin{aligned} H_1(\mathbf{J},n,N,\omega) &= -\frac{iZe}{\omega\tau_b}\int_0^{\tau_b} v_\perp\left[E_+ J_{n-1}(k_\perp\rho) + E_- J_{n+1}(k_\perp\rho)\right] e^{i\phi(t)} \\ d\phi/dt &= n\omega_c - \omega + \mathbf{k}\cdot\mathbf{v}_g \end{aligned} \quad (17)$$

where E_+ and E_- are the left- and right-hand polarized components of $\mathbf{E}$, respectively, $k_\perp$ is the component of the local wave vector $\mathbf{k}$ perpendicular to the background magnetic field, ρ is the Larmor radius, and $\mathbf{v}_g$ refers to the velocity of the guiding center. Usually, the integral in (17) can be evaluated by means of the stationary-phase method. It should be noted that n^2 does not appear in (17); it has

been eliminated by using the resonance condition (i.e. the delta function $\delta(\omega - \mathbf{n}\cdot\Omega)$) in (15).

IV. MONTE-CARLO OPERATORS

A. General considerations

In the Monte-Carlo approach, the Fokker-Planck equation is replaced by an equivalent Langevin equation, and a Monte-Carlo operator is formed which gives the particles random kicks with appropriate magnitudes and directions. As mentioned in the introduction, it is advantageous to do this for the orbit-averaged kinetic equation directly, rather than applying a local operator at a number of times each turn around the orbit, as was done in earlier Monte-Carlo studies[7,17]. This is true even if the operator for the averaged equation involves orbit-averages and thus requires an orbit integral to be calculated. The main reason is that the orbit integrals may be evaluated and tabulated on a grid in invariant-space at the beginning of the simulation. Subsequently, the value of these integrals for an arbitrary set of invariants can be obtained by interpolation[19]. Furthermore, the Monte-Carlo operators for the orbit-averaged equation needs to be applied fewer times than the local operators.

The purpose of this subsection is to derive general expressions for the mean values and covariances of the time variations which the invariants are subject to. In subsection B, we restrict the choice of invariants somewhat, and in the last subsection, we perform the actual construction of the Monte-Carlo operators.

As shown in Sec.II and III, the averaged kinetic equation has the form

$$\frac{\partial f_0}{\partial t} = g^{-1/2}\frac{\partial}{\partial I^i}\left[g^{1/2}\left(a^i f_0 + d^{ij}\frac{\partial f_0}{\partial I^j}\right)\right] \tag{18}$$

where a^i and d^{ij} are orbit-averaged quantities. In order to construct Monte-Carlo operators for this equation, one has to determine how a volume element in I-space evolves in time. In other words, one must calculate the time behavior of a distribution function of the form $f_0(\mathbf{I},t_0) = g^{-1/2}\delta(\mathbf{I}-\mathbf{I}_0)$. Defining the ensemble average $\langle\langle\cdots\rangle\rangle$ by

$$\langle\langle\cdots\rangle\rangle = \int(\cdots)f_0(\mathbf{I},t)g^{1/2}d^3I \tag{19}$$

we introduce the expectation values μ^i and covariances σ^{ij} for the invariants as

$$\begin{aligned}\mu^i &= << I^i >> \\ \sigma^{ij} &= << \left(I^i - \mu^i\right)\left(I^j - \mu^j\right) >>\end{aligned} \tag{20}$$

As follows from Eq.(18), the time derivative taken at $t=t_0$ of an arbitrary function of invariants, F(I), is

$$\left.\frac{dF(I)}{dt}\right|_{t=t_0} = -a^i \frac{\partial F}{\partial I^i} + g^{-1/2} \frac{\partial}{\partial I^j}\left(g^{1/2} d^{ij} \frac{\partial F}{\partial I^i}\right) \tag{21}$$

In particular, we have

$$\begin{aligned}d\mu^i / dt &= -a^i + g^{-1/2} \frac{\partial}{\partial I^j}\left(g^{1/2} d^{ij}\right) \\ d\sigma^{ij} / dt &= d^{ij} + d^{ji} = 2d^{ij}\end{aligned} \tag{22}$$

These equations describe the convection and spreading of a volume element in the space of constants of motion. Suitable interpreted, Eq.(22) contains exactly the same information as does the kinetic equation (18).

B. Choice of invariants

Up to this point, no restrictions have been placed on the invariants **I**; they could be any constants of motion. In the following, we shall restrict the discussion to invariants of the form

$$\begin{aligned}I^1 &= I^1(v) \\ I^2 &= I^2(\chi, q) \\ I^3 &= I^3(v, \chi, q)\end{aligned} \tag{23}$$

Thus, I^1 is assumed to depend solely on the energy, I^2 on the pitch angle and the guiding-centre position, and I^3 may depend on all phase-space coordinates. These assumptions lead to considerable simplifications of the explicit expressions for (21)-(22).given below; yet they are sufficiently general to cover virtually all choices of invariants appearing the literature. For example, a frequently employed choice of invariants[27,28] is $I=(v,\Lambda,p_\varphi)$, where $\Lambda=\mu B_0/(mv^2/2)$ and B_0 is the magnetic field strength at the magnetic axis. Then $\partial v/\partial J^i = \Omega^i/mv$, $\partial\Lambda/\partial J^i = (\omega_{c0}\delta^{i1}-\Lambda\Omega^i)/H$, and $\partial p_\varphi/\partial J^i = \delta^{i3}$, where $\omega_{c0} = ZeB_0/m$, and δ^{ij} is the Kronecker

symbol. The Jacobian (9) becomes $g^{1/2} = v^3/(2ZeB_0\omega_b)$, and the components of the quasilinear diffusion tensor given by (12) and (15) are

$$D^{11} = \pi \sum_{\mathbf{n},\omega} \left(\frac{\omega}{mv} \right)^2 |H_1|^2 \delta(\omega - \mathbf{n}\cdot\Omega) \tag{24a}$$

$$D^{12} = \pi \sum_{\mathbf{n},\omega} \frac{\omega}{mv} \frac{\omega_{c0} n^1 - \Lambda\omega}{H} |H_1|^2 \delta(\omega - \mathbf{n}\cdot\Omega \tag{24b}$$

$$D^{13} = \pi \sum_{\mathbf{n},\omega} \frac{\omega n^3}{mv} |H_1|^2 \delta(\omega - \mathbf{n}\cdot\Omega) \tag{24c}$$

$$D^{22} = \pi \sum_{\mathbf{n},\omega} \left(\frac{\omega_{c0} n^1 - \Lambda\omega}{H} \right) |H_1|^2 \delta(\omega - \mathbf{n}\cdot\Omega) \tag{24d}$$

$$D^{23} = \pi \sum_{\mathbf{n},\omega} \frac{\omega_{c0} n^1 - \Lambda\omega}{H} |H_1|^2 \delta(\omega - \mathbf{n}\cdot\Omega) \tag{24e}$$

$$D^{33} = \pi \sum_{\mathbf{n},\omega} \left(n^3 \right)^2 |H_1|^2 \delta(\omega - \mathbf{n}\cdot\Omega) \tag{24f}$$

Again, in the case of ICRH at the n:th harmonic of the cyclotron frequency and a single toroidal wave number N, all terms in the sums in (24) vanish except the ones with n^1=n and n^3=N. In reality, the delta functions appearing in (24) are not sharp; they are broadened by collisions and nonliear effects[20,25,26]. In fact, they must overlap in order for the diffusion actually to take place. The summation over n^2 is then easily accomplished. The sum is merely replaced by an integral, which upon evaluation gives, simply, $1/\Omega^2$. Thus, in (24), we may perform the replacement

$$\sum_{\mathbf{n},\omega} \delta(\omega - \mathbf{n}\cdot\Omega) \rightarrow \frac{1}{\omega_b} \sum_{n,N,\omega} \tag{24g}$$

The expressions (24) serve as an example of how to calculate D^{ij} for a specific choice of invariants. However, in order to keep the following discussion as general as possible, we shall keep the choice of invariants general, only imposing the restrictions (23).

C. Explicit operators

Armed with the results (13) and (21)-(22), and assuming (23), we can now explicitly calculate the time derivatives of the expectation values μ^i and the covariances σ^{ij} due to collisions and quasilinear RF-interaction. They are

$$d\mu^1/dt = < -\frac{\partial I^1}{\partial v}A^v + \frac{1}{v^2}\frac{\partial}{\partial v}\left(v^2\frac{\partial I^1}{\partial v}T^{vv}\right) + \frac{\partial I^1}{\partial v}\frac{\partial T^{v\chi}}{\partial \chi} > + g^{-1/2}\frac{\partial}{\partial I^j}\left(g^{1/2}D^{1j}\right) \tag{25a}$$

$$d\mu^2/dt = < -\frac{\partial I^2}{\partial \chi}A^\chi + \frac{\partial}{\partial \chi}\left(\frac{\partial I^2}{\partial \chi}T^{\chi\chi}\right) + \frac{\partial I^2}{\partial \chi}\frac{1}{v^2}\frac{\partial}{\partial v}\left(v^2\frac{\partial T^{v\chi}}{\partial v}\right) > + g^{-1/2}\frac{\partial}{\partial I^j}\left(g^{1/2}D^{2j}\right) \tag{25b}$$

$$d\mu^3/dt = < -\frac{\partial I^3}{\partial v}A^v - \frac{\partial I^3}{\partial \chi}A^\chi + \frac{1}{v^2}\frac{\partial}{\partial v}\left[v^2\left(\frac{\partial I^3}{\partial v}T^{vv} + \frac{\partial I^3}{\partial \chi}T^{v\chi}\right)\right] + \frac{\partial}{\partial \chi}\left(\frac{\partial I^3}{\partial v}T^{v\chi} + \frac{\partial I^3}{\partial \chi}T^{\chi\chi}\right) > + g^{-1/2}\frac{\partial}{\partial I^j}\left(g^{1/2}D^{3j}\right) \tag{25c}$$

$$d\sigma^{11}/dt = 2\left(\partial I^1/\partial v\right)^2 < T^{vv} > + 2D^{11} \tag{25d}$$

$$d\sigma^{22}/dt = 2 < \left(\partial I^2/\partial \chi\right)^2 T^{\chi\chi} > + 2D^{22} \tag{25e}$$

$$d\sigma^{33}/dt = 2 < \left(\frac{\partial I^3}{\partial v}\right)^2 T^{vv} + 2\frac{\partial I^3}{\partial v}\frac{\partial I^3}{\partial \chi}T^{v\chi} + \left(\frac{\partial I^3}{\partial \chi}\right)^2 T^{\chi\chi} > + 2D^{33} \tag{25f}$$

$$d\sigma^{12}/dt = d\sigma^{21}/dt = 2\frac{\partial I^1}{\partial v} < \frac{\partial I^2}{\partial \chi}T^{v\chi} > + 2D^{12} \tag{25g}$$

$$d\sigma^{13}/dt = d\sigma^{31}/dt = 2\frac{\partial I^1}{\partial v} < \frac{\partial I^3}{\partial v}T^{vv} + \frac{\partial I^3}{\partial \chi}T^{v\chi} > + 2D^{13} \tag{25h}$$

$$d\sigma^{23}/dt = d\sigma^{32}/dt = 2 < \frac{\partial I^2}{\partial \chi}\left(\frac{\partial I^3}{\partial v}T^{v\chi} + \frac{\partial I^3}{\partial \chi}T^{\chi\chi}\right) > + 2D^{23} \tag{25i}$$

In the case of test-particle interaction with a Maxwellian background, these expressions are further simplified by the use of (A2)-(A4).

Monte-Carlo operators, representing a random walk in I-space with a time-step Δt, are now given by changing the values of the invariants I^i at the n:th step to those at the next step according to

$$I^i_{n+1} = I^i_n + \Delta I^i \tag{26}$$

where the quantities ΔI^i are stochastic variables whose expectation values and covariances are given by

$$\begin{aligned} E\left[\Delta I^i\right] &= \left(d\mu^i / dt\right)\Delta t \\ C\left[\Delta I^i, \Delta I^j\right] &= \left(d\sigma^{ij} / dt\right)\Delta t \end{aligned} \tag{27}$$

In order to construct ΔI^i, we utilize the fact that the covariance matrix $C[\Delta I^i,\Delta I^j]$ is symmetric and positive definite[29]. Therefore, it can be diagonalized, i.e. there exists a unitary matrix M such that

$$C\left[\Delta I^i, \Delta I^j\right] = M^{ik}\Lambda^{kl}M^{jl} \tag{28}$$

where $\Lambda^{kl} = \mathrm{diag}(\lambda^1,\lambda^2,\lambda^3)$ is the diagonal matrix of the eigenvalues. Since the latter are positive, we may introduce the matrix $L^{kl} = \mathrm{diag}[(\lambda^1)^{1/2},(\lambda^2)^{1/2},(\lambda^3)^{1/2}]$, and write the covariance matrix as

$$C\left[\Delta I^i, \Delta I^j\right] = M^{ik}L^{km}L^{lm}M^{jl} \tag{29}$$

From this relation, it follows that the conditions (27) are satisfied if ΔI^i is chosen as

$$\Delta I^i = \left(d\mu^i / dt\right)\Delta t + M^{ik}L^{kl}\xi^1 \tag{30}$$

where ξ^1 are arbitrary, uncorrelated, stochastic variables with vanishing expectation values and unit variances. For instance, we may choose $\xi^1 = \pm 1$ with equal probabilities. This completes the construction of the Monte-Carlo operators. The final results are displayed in Eqs (25),(26) and (30). The diagonalization procedure used to form ΔI^i may be intuitively pictured as a rotation in I-space to some fundamental direction in which the random kicks given to the invariants are orthogonal and independent. Recently, an alternative construction of ΔI^i from the covariance matrix has been given by Putvinskij et al.[19].

V. CONCLUSIONS

In this paper, we have derived 3D Monte-Carlo operators for the orbit-averaged Fokker-Planck equation describing general collisional and quasilinear processes. All effects of orbit topology, such as large banana-width and non-standard orbit shape are taken into account. Although, we primarily focus on ICRH in tokamaks, the discussion has been kept as general as possible. We believe that the resulting operators should be widely useful since they have been derived under very general assumptions, but yet are given in a quite explicit form. For example, no appeal has been made to the specific geometry of a tokamak, except for the existence of action-angle variables. However, the detailed geometry must, of course, be taken into account once the orbit-averages appearing in the Monte-Carlo operators are performed. Since the Monte-Carlo operators are derived under such general assumptions, they may be used to simulate a broad range of phenomena, such as neoclassical transport, radio-frequency heating and wave-driven spatial diffusion in arbitrary axisymmetric magnetic configurations.

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APPENDIX: THE COLLISION OPERATOR

The components of the vector A and the tensor T appearing in the collision operator (13) have the general form[23]

$$A^v = \sum_s K_s \frac{\partial \varphi_s}{\partial v} \tag{A1a}$$

$$A^\chi = \sum_s K_s \frac{\partial \varphi_s}{\partial \chi} \tag{A1b}$$

$$T^{vv} = \sum_s K_s \frac{\partial^2 \psi_s}{\partial v^2} \tag{A1c}$$

$$T^{\chi\chi} = \sum_s K_s \frac{1-\chi^2}{v^2}\left(\frac{1-\chi^2}{v^2}\frac{\partial^2 \psi_s}{\partial \chi^2} - \frac{\chi}{v^2}\frac{\partial \psi_s}{\partial \chi} + \frac{1}{v}\frac{\partial \psi_s}{\partial v}\right) \tag{A1d}$$

$$T^{v\chi} = T^{\chi v} = -\sum_s K_s \frac{1-\chi^2}{v^2}\left(\frac{\partial^2 \psi_s}{\partial v \partial \chi} - \frac{1}{v}\frac{\partial \psi_s}{\partial \chi}\right) \tag{A1e}$$

Here, $K_s = \left(4\pi Z Z_s e^2 / m^2\right)$, $\ln \Lambda_s$ is the Coulomb logariathm, the sums should be taken over all particle species s, and the potentials φ_s and ψ_s, introduced by Trubnikov[24], are given by

$$\begin{aligned} \varphi_s(\mathbf{v}) &= -\frac{1}{4\pi}\int \frac{f_s(\mathbf{v}')}{|\mathbf{v}-\mathbf{v}'|} d^3v' \\ \psi_s(\mathbf{v}) &= -\frac{1}{8\pi}\int |\mathbf{v}-\mathbf{v}'| f_s(\mathbf{v}') d^3v' \end{aligned} \tag{A2}$$

Frequently, all species s included in the sums are Maxwellian, except for the hot minority species, among which self-collisions may be neglected. Then the expressions for the components of A and T simplify to[25]

$$A^v = -\alpha + \frac{1}{2v^2}\frac{\partial}{\partial v}\left(\beta v^2\right) \tag{A3a}$$

$$T^{vv} = \beta / 2 \tag{A3b}$$

$$T^{v\chi} = \gamma\left(1-\chi^2\right)/4v^2 \tag{A3c}$$

$$A^{\chi} = 0, T^{v\chi} = 0 \tag{A3d}$$

where

$$\alpha(\mathbf{q},\mathbf{v}) = -\sum_s \left[C_s 1_s^2 (1 + m/m_s) G(1_s v) + \gamma(\mathbf{q},\mathbf{v})/2v\right] \tag{A4a}$$

$$\beta(\mathbf{q},\mathbf{v}) = \sum_s C_s G(1_s v)/v \tag{A4b}$$

$$\gamma(\mathbf{q},\mathbf{v}) = \sum_s C_s \left[\Phi(1_s v) - G(1_s v)\right]/v \tag{A4c}$$

Here $C_s(\mathbf{q}) = 8\pi n_s Z_s^2 Z^2 e^4$, $1_s = (m/2kT_s)^{1/2}$, Φ is the error function, and $G(x) = [\Phi(x) - \Phi'(x)]/2x^2$.

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