Solution of the drift kinetic equation in the regime of weak collisions by stochastic mapping techniques

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A new method for solving the drift kinetic equation applicable for non-integrable particle motion is presented. To obtain this goal, the general form of the drift kinetic equation is reduced to a stochastic mapping equation which is valid in the weak collisions regime. This equation describes the evolution of the distribution function on Poincaré cuts of phase space. The proposed Monte Carlo algorithm applied to the stochastic mapping equation turns out to solve the drift kinetic equation much faster than a direct integration of stochastic orbits. It can be applied to study quasilinear effects of radio frequency heating and transport in systems with complex magnetic field geometries such as stellarators, tokamaks with toroidal magnetic field ripples, or ergodic divertors. For systems with axial space symmetry the stochastic mapping equation is shown to reduce to the well-known canonical (bounce) averaged equation. For nonaxisymmetric magnetic fields the bounce averaged equation for trapped particles is recovered. © *1997 American Institute of Physics.* [S1070-664X(97)02107-1]

I. INTRODUCTION

In studies of plasma confinement and heating in magnetic traps one needs to know the evolution of the ''unperturbed'' part of the particle distribution function which evolves on a slow time scale of the order of collision time or even longer. This function satisfies the drift kinetic equation including quasilinear contributions from different rf heating mechanisms and possible sources and sinks in phase space due to beam injection, etc. The high dimensionality of the problem makes it difficult to solve it in a straightforward way with regular methods without the reduction of the dimensionality. However, such a reduction is not always possible, and therefore Monte Carlo (MC) methods[1–10] which are much less sensitive with respect to number of dimensions are used.

In the case of weak collisions, a direct application of the MC method to the solution of this drift kinetic equation,[1,2,5,8–10] i.e., the modeling of stochastic guiding center trajectories, suffers from the need to cover simultaneously two different time scales, the ''fast'' bounce time corresponding to unperturbed motion which enters the equation through a dynamic convection term, and the ''slow'' collisional relaxation time which is determined by ''collisional'' terms, i.e., the Coulomb collision integral, the quasilinear diffusion operator, and sources and sinks. The time step for the MC integration has to be much smaller than the bounce time, whereas the total integration time should be much larger than the collisional relaxation time or, even worse, the transport time in the case of balance-type problems, in this context being defined as problems which require the computation of the distribution function in the whole phase space in contrast to the problem of computing the transport coefficients when the kinetic equation can be solved only locally[2] and, at the same time, linearization can be used.[9,10] As a consequence, the problem becomes numerically stiff. Because of this stiffness, balance-type problems, such as the modeling of minority ion distributions during cyclotron heating,[5,8] can be solved with direct methods only with the help of supercomputers. In the case of an exactly or approximately integrable system for free particle motion, the stiffness problem can be resolved by averaging the kinetic equation over canonical angles and, at the same time, the number of dimensions can be reduced to the number of the remaining canonical action variables[11] or to the equivalent noncanonical integrals of motion. For systems with axial symmetry such as tokamaks these invariants are the total energy, magnetic moment, and generalized toroidal moment, where the first and the last one are preserved exactly.

For systems with broken symmetry such as stellarators or tokamaks with toroidal magnetic field ripples, the toroidal moment is not preserved anymore. However, the dynamics will be still approximately integrable if one exploits the difference in time scales for the motion across the magnetic field ripples and the poloidal revolution to perform ripple (trapped-bounce) averaging. In particular, for trapped particles the difference in bounce time and time of trapped orbit drift as a whole can be used to remove the rapid bounce motion from the equation for these particles by averaging over the fast bounce phase, see, e.g., Refs. 3 and 4. In this case, the relatively slow drift motion which preserves the ''parallel'' adiabatic invariant survives averaging.

Even more approximate similar procedures applied to passing particles in stellarators (to this set also the toroidally trapped particles are counted for in the stellarator literature), namely averaging the kinetic equation over helical ripples,[12,13] also relaxes the stiffness of the problem in re-

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moving rapid oscillations of particle phase space coordinates associated with the ripples. Here, the difference between the time to pass a single ripple and the period of poloidal motion or, in other words, the smallness of rotational transform per one ripple, is used. The adiabatic invariant associated with this double time scale[14,15] demonstrates the integrability of motion also in this case.

MC algorithms based on the bounce and canonically averaged equations[3,4,6,7] are much more effective than direct methods because the step size of time integration of the stochastic orbits in averaged methods is much larger than the bounce time. For axially symmetric systems, together with canonical averaging, often methods are used which are not based on a Hamiltonian formalism, see, e.g., Ref. 16. Because the resulting equation is basically the same, in the context of this paper the term ''canonical averaging'' will be used for all such approaches which completely remove the unperturbed motion from the equation. They are also often referred to as ''bounce averaging,'' however, this term will be used here for those methods where only the averaging over parallel bounce motion is performed. The maximum efficiency is gained in canonically averaged methods where just the collision time scale has to be met.

Note that the stiffness is not completely removed by bounce or ripple-averaging. The ripple-averaged equations have a stiffness similar to the tokamak problem. For bounce averaged motion of trapped particles in the case of very rare collisions, the time scale of particle drift may also become much shorter than the collision time and again a stiffness problem appears. The further reduction of stiffness is possible if one makes use of the parallel or ripple invariants in order to make the system fully integrable. This is a somewhat demanding task because the invariant surfaces are complex and there also exist transiting particles for which the invariants are not preserved all the time and one has to calculate appropriate transition probabilities.[14,15] Note that the need of transition probabilities already appears in the ripple-averaged equations irrespective of further averaging. On the other hand, ripple averaging requires the existence of nested flux surfaces as well as the equivalence of all helical ripples. But this might be destroyed, e.g., when magnetic islands or ergodic layers are present in the configuration or by a localized heating of the plasma with rf heating methods.

Therefore, it is desirable to develop a general procedure in which the computer time for modeling the regular particle motion is minimized down to the amount actually required for modeling the stochastic process and, at the same time, allows one to treat cases with destroyed magnetic surfaces and dynamically unstable orbits.

In the present paper a procedure based on Poincaré mapping techniques is proposed which seems to meet all the goals discussed. It takes full advantage of the mapping procedure describing the unperturbed motion and, at least in the ideal case, one mapping step is sufficient to cover any desired time interval. For purely deterministic motion these techniques are well established in fusion studies, e.g., in modeling of magnetic surfaces[17] or cyclotron heating in nonuniform magnetic fields.[18,19] Also, stochastic processes have been included in simple models using some kind of mapping procedure.[20] The method proposed in the present paper allows for a rigorous account of stochastic diffusion processes during the mapping in realistic magnetic field geometries and weakly collisional plasmas.

The structure of the paper is the following. In Section II, using exact constants of motion, a Poincaré map is constructed and, with its help, for the regime of weak collisions a stochastic mapping equation (SME) for the particle flux density through the Poincaré cuts is derived. In a first step, single-pass mapping is considered. In Section III a Monte Carlo algorithm is introduced which is able to solve the problem much faster than any method based on direct integration of the stochastic particle orbits. In Section IV it is shown how to compute the map-associated diffusion coefficients. In Section V, based on the single-pass SME, a multipass stochastic mapping procedure is developed. The efficiency of the Monte Carlo algorithms based on this multipassing procedure is close to the efficiency of canonically averaged methods. In Section VI expressions for averaged quantities in terms of the solution of the SME are given. In Section VII the SME is simplified for the phase space regions of trapped particles and the result is shown to be equivalent to the bounce averaged equation. For systems with axial space symmetry the canonically averaged equation is recovered from the SME and validity conditions for the full canonical averaging procedure are discussed. Finally, the results are discussed and summarized in the concluding section.

II. SINGLE-PASS MAPPING

In kinetic theory, the dynamics of the distribution function $f(t,\boldsymbol{z})$ in any system of dynamical variables $\boldsymbol{z}$ invertibly related to Cartesian variables $(\boldsymbol{r},\boldsymbol{p})$ obeys the equation

$$\frac{\partial f}{\partial t}+V^{\alpha}\frac{\partial f}{\partial z^{\alpha}}=\frac{1}{J}\frac{\partial}{\partial z^{\alpha}}J\left(D^{\alpha\beta}\frac{\partial f}{\partial z^{\beta}}-F^{\alpha}f\right)-\nu_0 f+Q,$$
$$\alpha=1\cdots 6. \tag{1}$$

Here, V^{α} is the phase space velocity of dynamic convection, $D^{\alpha\beta}$ and F^{α} are the components of the (properly transformed contravariant) collisional diffusion tensor and friction force including quasilinear contributions from the interaction with the waves, $1/\nu_0$ is the particle lifetime due to inelastic processes, Q represents possible sources and sinks in phase space, and J is the Jacobian of the transformation from Cartesian variables $(\boldsymbol{r},\boldsymbol{p})$ to some general new variables $\boldsymbol{z}\equiv(\boldsymbol{x},\boldsymbol{y})$ in 6-D phase space,

$$J=\frac{\partial(r_1,r_2,r_3,p_1,p_2,p_3)}{\partial(x^1,x^2,x^3,y^1,y^2,y^3)}. \tag{2}$$

For studies of processes with length and time scales much larger than the gyroradius and inverse gyrofrequency, an appropriate choice for the dynamical variables $(\boldsymbol{x},\boldsymbol{y})$ are guiding center variables. For the method developed below it is convenient to use the formulation introduced in Refs. 21 and 22, i.e., guiding center variables such that the resulting system conserves energy and phase space volume exactly (Hamiltonian system). On the other hand, the parallel guiding center world velocity $U_{\|}$ and magnetic moment μ used

in Ref. 22 are not very convenient to deal with the Coulomb collision operator. Therefore some new variables $\boldsymbol{y}=(p,\lambda,\phi)$ implicitly defined through

$$U_{\parallel}=\frac{p\lambda}{m_0},\quad \mu=\frac{p^2(1-\lambda^2)}{2m_0B},\quad \Theta=\phi, \tag{3}$$

will be used where m_0 is the rest mass and ϕ the gyrophase. One should note that the variables p and λ defined in this way are not the actual particle momentum module $|\boldsymbol{p}|$ and pitch angle cosine $\boldsymbol{B}\cdot\boldsymbol{p}/|\boldsymbol{B}||\boldsymbol{p}|$ but may differ from them by first-order terms in the guiding center expansion. However, this difference can be neglected when used in the collision term because this effect itself is of higher order.

Let $\boldsymbol{R}$ be the guiding center position in Cartesian coordinates and $\boldsymbol{x}=(x^1,x^2,x^3)$ be its position in some general curvilinear space coordinate system. Then the Jacobian (2) becomes

$$J=J_xJ_y,\quad J_x\equiv\sqrt{g}=\det\left(\frac{\partial R_i}{\partial x^j}\right),$$
$$J_y=\frac{\partial(\boldsymbol{p},\boldsymbol{r})}{\partial(\boldsymbol{y},\boldsymbol{R})}=\frac{B_{\parallel}^*(\boldsymbol{z})}{B(\boldsymbol{x})}p^2, \tag{4}$$

where[22,23]

$$B_{\parallel}^*(\boldsymbol{z})=\frac{B_iB^{*i}}{B},\quad B^{*i}=B^i+\frac{c}{e}\frac{p\lambda}{\sqrt{g}}\varepsilon^{ijk}\frac{\partial}{\partial x^j}\left(\frac{B_k}{B}\right). \tag{5}$$

Here, e, c, B^i, and B_i, are particle charge, speed of light, contra and covariant components of the magnetic field, respectively, and ε^{ijk} is the completely antisymmetric unit tensor (Levi-Civita symbol).

Introducing the relativistic factor, cyclotron frequency, and parallel velocity,

$$\gamma=\sqrt{1+\frac{p^2}{m_0^2c^2}},\quad \omega_c=\frac{eB}{m_0c\gamma},\quad v_{\parallel}=\frac{\lambda p}{m_0\gamma}, \tag{6}$$

the system governing the dynamics of ''free'' particle motion in stationary electric and magnetic fields becomes,

$$\frac{d}{dt}x^i=V^i=v_g^i,\quad i=1,\ldots,3, \tag{7}$$

$$\frac{d}{dt}p=V^4=-em_0\frac{\gamma}{p}v_g^i\frac{\partial\varphi}{\partial x^i}, \tag{8}$$

$$\frac{d}{dt}\lambda=V^5=-\frac{1-\lambda^2}{\lambda}\left(em_0\frac{\gamma}{p^2}v_g^i\frac{\partial\varphi}{\partial x^i}+\frac{1}{2}v_g^i\frac{\partial\ln B}{\partial x^i}\right), \tag{9}$$

$$\frac{d}{dt}\phi=V^6=-\omega_c, \tag{10}$$

with the contravariant guiding center velocity given by

$$v_g^i=\frac{1}{B_{\parallel}^*}\left(v_{\parallel}B^{*i}+\varepsilon^{ijk}\frac{cB_j}{B\sqrt{g}}\left(\frac{\partial\varphi}{\partial x^k}+\frac{\mu}{e\gamma}\frac{\partial B}{\partial x^k}\right)\right). \tag{11}$$

Here, φ is the electrostatic potential and $v_{\parallel}$ as well as μ are to be expressed through p and λ using (6) and (3), respectively.

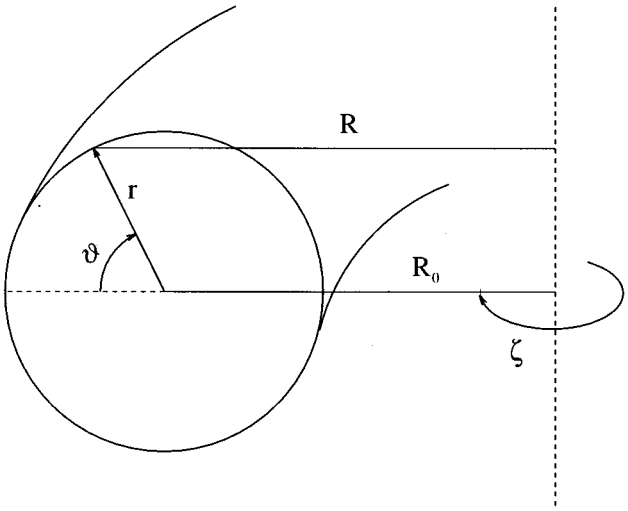

FIG. 1. Quasitoroidal coordinate system.

In the particular case of a tokamak with circular concentric magnetic surfaces, a convenient choice of space coordinates x^i is quasitoroidal coordinates $x^i=(\zeta,r,\vartheta)$, where ζ,r,ϑ are the toroidal angle, the small radius, and the poloidal angle (see Fig. 1). For this set of coordinates

$$J_x=rR,\quad R=R_0+r\cos\vartheta, \tag{12}$$

where R_0 is the big radius of the magnetic axis.

In the following it will be convenient to use such a system of space variables $(x^1,x^2,x^3\equiv\vartheta)$ in which one magnetic field component, say B^{ϑ}, is positive definite everywhere in the considered volume. Below it will be shown how the problem can be discretized with respect to this coordinate. In the tokamak geometry introduced above, the poloidal angle $x^3=\vartheta$ will serve for this purpose. Defining the remaining set of variables by $\boldsymbol{u}=(x^1,x^2,p,\lambda)$, the interesting subset of equations of motion (7)–(10) can be written as

$$\frac{d}{dt}\vartheta=\Omega(\vartheta,\boldsymbol{u}),\quad \frac{d}{dt}u^i=w^i(\vartheta,\boldsymbol{u}),\quad i=1,\ldots,4. \tag{13}$$

Clearly, the system is Hamiltonian and obeys Liouville's theorem,

$$\frac{1}{J}\frac{\partial}{\partial z^{\alpha}}JV^{\alpha}=\frac{1}{J}\left(\frac{\partial}{\partial\vartheta}J\Omega+\frac{\partial}{\partial u^i}Jw^i\right)=0. \tag{14}$$

Let the flow, i.e., the set of trajectories for all possible initial conditions, generated by vector field $(\Omega,\boldsymbol{w})$ of (13) be denoted by

$$\vartheta=\Theta(\tau,\vartheta_0,\boldsymbol{u}_0),\quad \Theta(0,\vartheta_0,\boldsymbol{u}_0)=\vartheta_0,$$
$$u^i=U^i(\tau,\vartheta_0,\boldsymbol{u}_0),\quad U^i(0,\vartheta_0,\boldsymbol{u}_0)=u_0^i, \tag{15}$$

such that

$$\frac{\partial}{\partial\tau}\Theta(\tau,\vartheta_0,\boldsymbol{u}_0)=\Omega(\Theta(\tau,\vartheta_0,\boldsymbol{u}_0),\boldsymbol{U}(\tau,\vartheta_0,\boldsymbol{u}_0)),$$
$$\frac{\partial}{\partial\tau}U^i(\tau,\vartheta_0,\boldsymbol{u}_0)=w^i(\Theta(\tau,\vartheta_0,\boldsymbol{u}_0),\boldsymbol{U}(\tau,\vartheta_0,\boldsymbol{u}_0)). \tag{16}$$

Obviously, solutions (15) of the equations of motion satisfy the group property

$$\Theta(\tau_1,\Theta(\tau_2,\vartheta_0,\boldsymbol{u}_0))=\Theta(\tau_1+\tau_2,\vartheta_0,\boldsymbol{u}_0),$$
$$\boldsymbol{U}(\tau_1,\boldsymbol{U}(\tau_2,\vartheta_0,\boldsymbol{u}_0))=\boldsymbol{U}(\tau_1+\tau_2,\vartheta_0,\boldsymbol{u}_0). \tag{17}$$

With the help of these trajectories, Poincaré maps will be constructed with respect to hypersurfaces in phase space. If the initial values $(\vartheta_0,\boldsymbol{u}_0)$ in (15) are restricted to lie within a hypersurface (labeled by m) of phase space defined through the relation

$$\vartheta-\vartheta_{(m)}(\boldsymbol{u})=0, \tag{18}$$

with some function $\vartheta_{(m)}(\boldsymbol{u})$ such that the integral lines of (13) always intersect the surface with a finite angle, i.e., the surface should be transverse to the vector field $(\Omega,\boldsymbol{w})$ everywhere, it is possible to introduce a set of Lagrangian type variables $(\tau,\boldsymbol{u}_m)$ related to the old variables $(\vartheta,\boldsymbol{u})$ by

$$\vartheta=\Theta(\tau,\vartheta_{(m)}(\boldsymbol{u}_m),\boldsymbol{u}_m)\equiv\hat{\Theta}(\tau,\boldsymbol{u}_m),$$
$$\hat{\Theta}(0,\boldsymbol{u}_m)=\vartheta_{(m)}(\boldsymbol{u}_m),$$
$$u^i=U^i(\tau,\vartheta_{(m)}(\boldsymbol{u}_m),\boldsymbol{u}_m)\equiv\hat{U}^i(\tau,\boldsymbol{u}_m),\quad \hat{U}^i(0,\boldsymbol{u}_m)=\boldsymbol{u}_m. \tag{19}$$

Note that subscript m is not a covariant index but indicates the new set of variables related to the hypersurface with number m.

From the group property (17), it follows

$$\vartheta_{(m)}(\boldsymbol{u}_m)=\Theta(-\tau,\vartheta,\boldsymbol{u}),$$
$$u^i_m=U^i(-\tau,\vartheta,\boldsymbol{u}). \tag{20}$$

Through the coordinates change from $(\vartheta,\boldsymbol{u})$ to $(\tau,\boldsymbol{u}_m)$, the contravariant velocity is rectified, i.e., $V^\alpha_m=(1,0,0,0,0)$ and the equations of motion simply become

$$\frac{d\tau}{dt}=1,\quad \frac{du^i_m}{dt}=0. \tag{21}$$

The complete Jacobian from Cartesian to Lagrangian variables is

$$J_m(\tau,\boldsymbol{u}_m)\equiv J(\vartheta,\boldsymbol{u})\frac{\partial(\vartheta,\boldsymbol{u})}{\partial(\tau,\boldsymbol{u}_m)}. \tag{22}$$

Evaluating this expression in the limit $\tau\to0$ and taking into account (19) and (16), it follows for the Jacobian,

$$J_m=J(\vartheta_{(m)}(\boldsymbol{u}_m),\boldsymbol{u}_m)\Big(\Omega(\vartheta_{(m)}(\boldsymbol{u}_m),\boldsymbol{u}_m)$$
$$-w^i(\vartheta_{(m)}(\boldsymbol{u}_m),\boldsymbol{u}_m)\frac{\partial\vartheta_{(m)}}{\partial u^i_m}\Big), \tag{23}$$

valid for arbitrary τ because from Liouville's theorem (14), the Jacobian must be independent on τ,

$$\frac{\partial}{\partial\tau}J_m=0. \tag{24}$$

On the other hand, as sketched in Appendix A, the velocity flux through the area element d^4u_m of the hypersurface (18) is given by

$$V^\alpha(dS)_\alpha=JV^\alpha\frac{\partial}{\partial z^\alpha}(\vartheta-\vartheta_{(m)}(\boldsymbol{u}))\Big|_{\boldsymbol{u}=\boldsymbol{u}_m}du^1_m\cdots du^4_m$$
$$=J\left(\frac{\partial}{\partial\tau}\,(\hat{\Theta}(\tau,\boldsymbol{u}_m)-\vartheta_{(m)}(\hat{\boldsymbol{U}}(\tau,\boldsymbol{u}_m)))\right)\Big|_{\tau=0}$$
$$\times du^1_m\cdots du^4_m=J_m du^1_m\cdots du^4_m. \tag{25}$$

Therefore, the Jacobian is identical to the velocity flux density through the hypersurface and will be nonzero if the surface is never tangent to the characteristics of the kinetic equation. This, in turn, is the definition of such a hypersurface which will be used as a Poincaré cut for discretization of the unperturbed particle motion. The choice of this surface is not unique and the envisaged geometry should be a guide to finding a topology as simple as possible. For systems with limited particle motion in phase space, e.g., magnetic traps, the number of Poincaré cuts necessary to cover all particle populations is finite, say $m_{\max}$. Subscript m will be used to number these cuts, such that m is increasing in the direction of the magnetic field and is periodic with the period $m_{\max}$, $m+m_{\max}\to m$, i.e., the cut with number $m+m_{\max}$ is the same as the cut with number m. For magnetic traps without stationary parallel electric field, a good choice for the hypersurface is magnetic field minimum surfaces defined by

$$\boldsymbol{B}(\boldsymbol{r})\cdot\nabla B(\boldsymbol{r})=B^i(\boldsymbol{x})\frac{\partial B(\boldsymbol{x})}{\partial x^i}=0. \tag{26}$$

Such a Poincaré cut imposes no restrictions on momentum space variables.

For example, for the tokamak model introduced above, just one surface is sufficient if the equatorial cross section defined by $\vartheta=0$ (see Fig. 1) is used, i.e., the period is $m_{\max}=1$. In the lowest-order guiding center approximation, the Jacobian turns out to be

$$J_m=h^\vartheta p^2 rRv_\parallel=\frac{B_{\langle\vartheta\rangle}}{B}p^3R\frac{\lambda}{\gamma m}\Big|_{\vartheta=0}, \tag{27}$$

where $B_{\langle\vartheta\rangle}$ is the physical poloidal component of the magnetic field and the values

$$u^1_m=r,\quad u^2_m=\zeta,\quad u^3_m=p,\quad u^4_m=\lambda \tag{28}$$

have to be taken on the Poincaré cut $m=1$.

In the new variables $(\tau,\boldsymbol{u}_m)$, the kinetic equation (1) becomes

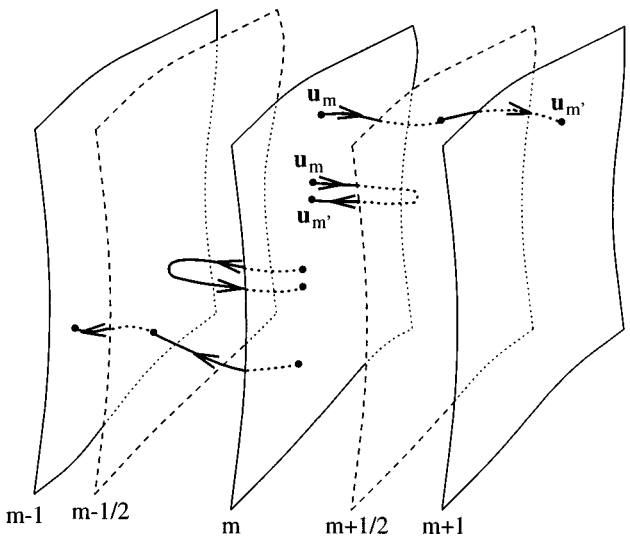

FIG. 2. Different types of particle trajectories. On top pointing to the right a copassing orbit, next two different trapped orbits, at the bottom pointing to the left a counterpassing orbit. The surfaces $m-1$, m, and $m+1$ are Poincaré cuts. The surfaces $m-1/2$ and $m+1/2$ indicate separatrix surfaces.

$$\frac{\partial f}{\partial \tau}=\frac{\partial}{\partial \tau}\left(D_m^{\tau\tau}\frac{\partial f}{\partial \tau}+D_m^{\tau j}\frac{\partial f}{\partial u_m^j}-F_m^{\tau}f\right)+\frac{1}{J_m}\frac{\partial}{\partial u_m^i}J_m\left(D_m^{i\tau}\frac{\partial f}{\partial \tau}+D_m^{ij}\frac{\partial f}{\partial u_m^j}-F_m^i f\right)-\frac{\partial f}{\partial t}-\nu_0 f+Q, \tag{29}$$

where the components of collisional diffusion tensor and friction force have to be transformed according to the rules of tensor algebra,

$$D_m^{ij}(\tau,\boldsymbol{u}_m)=\overline{c}^{\,i}_{\,k}\overline{c}^{\,j}_{\,l}D^{kl}(\vartheta,\boldsymbol{u}), \tag{30}$$

$$F_m^i(\tau,\boldsymbol{u}_m)=\overline{c}^{\,i}_{\,k}F^k(\vartheta,\boldsymbol{u}). \tag{31}$$

with the transformation matrix given by $[\boldsymbol{z}^i\equiv(\vartheta,\boldsymbol{u})]$

$$\overline{c}^{\,\tau}_{\,k}=\frac{\partial \tau}{\partial z^k},\quad \overline{c}^{\,i}_{\,k}=\frac{\partial u_m^i}{\partial z^k},\quad i=1,\ldots,4. \tag{32}$$

Let a ''bounce'' time $\tau_b(\boldsymbol{u}_m)$ (time for the transition of the particle from the initial Poincaré cut m to the next Poincaré cut m' the particle hits on its path) be defined as the smallest positive root of the equation

$$\vartheta_{m'}(\hat{\boldsymbol{U}}(\tau,\boldsymbol{u}_m))=\hat{\Theta}(\tau,\boldsymbol{u}_m) \tag{33}$$

with respect to τ variable. The particles can now be grouped into three classes with respect to the mapping from the cut m to the cut m'. The corresponding orbits of co-passing particles with $m'=m+1$, counter-passing particles with $m'=m-1$, and particles reflected from the magnetic mirror with $m'=m$ are shown in Fig. 2. In the present context, any particle which is reflected by the magnetic field mirror between neighboring Poincaré cuts will be called trapped. This definition also includes particles trapped in the usual sense, i.e., those returning to the same cut twice without intersecting the neighboring cuts. They will be referred to as ''strictly trapped'' particles and their oscillation period is twice the ''bounce'' time defined above. In stellarator literature, often just that type of particles are called trapped while the other kinds of trapped particles are referred to as passing. Also shown in Fig. 2 are hypersurfaces which divide the phase space into regions containing trapped particles with start and end points on the same Poincaré cut m. These surfaces are numbered with index $m\pm 1/2$ and all trapped particles whose coordinate θ satisfies $\vartheta_{m-1/2}<\vartheta<\vartheta_{m+1/2}$ belong to the cut m. For the case of zero parallel electric field, these surfaces up to zero order in the drift approximation coincide with magnetic field maximum surfaces which also satisfy (26).

The variables $(\tau,\boldsymbol{u}_m)$ associated with the Poincaré cut m are related to the variables $(\tau',\boldsymbol{u}_{m'})$ of the aligned Poincaré cut m' as

$$\tau'=\tau-\tau_b(\boldsymbol{u}_m), \tag{34}$$

$$u^i_{m'}=\hat{U}^i(\tau_b(\boldsymbol{u}_m),\boldsymbol{u}_m)\equiv\hat{U}^i_m(\boldsymbol{u}_m). \tag{35}$$

With the help of functions (35), the unperturbed motion on time scales long compared to the bounce time can be replaced by the mapping from one Poincaré cut to another and thereby discretized. In the particular case of a tokamak, the set of mapping functions for passing particles $\hat{U}^i_m$ with the definitions (28) becomes

$$r_{m'}=\hat{U}^1_m(\boldsymbol{u}_m)=r_m, \tag{36}$$

$$\zeta_{m'}=\hat{U}^2_m(\boldsymbol{u}_m)=\zeta_m+2\pi q\ \mathrm{sgn}\ \lambda_m+\Delta\zeta(\lambda_m,p_m,r_m), \tag{37}$$

$$p_{m'}=\hat{U}^3_m(\boldsymbol{u}_m)=p_m, \tag{38}$$

$$\lambda_{m'}=\hat{U}^4_m(\boldsymbol{u}_m)=\lambda_m. \tag{39}$$

Here, q is the safety factor and $\Delta\zeta$ is the toroidal orbit shift due to electric and magnetic drift per mapping. For banana particles the mapping over toroidal angle is given by (37) without the second term in the right-hand side, while the rest of the mapping functions have a more complicated form because only half of the rotation period along the banana orbit corresponds to the ''bounce'' time. However, after two mappings they again satisfy

$$\hat{U}^i{}_m(\boldsymbol{U}_m(\boldsymbol{u}_m))=u^i_m,\quad i=1,3,4. \tag{40}$$

Integrating the kinetic equation (29) over a bounce period leads to

$$f|_{\tau=\tau_b}J_m-f|_{\tau=0}J_m=\left[D_m^{\tau\tau}\frac{\partial f}{\partial \tau}+D_m^{\tau j}\frac{\partial f}{\partial u_m^j}-F_m^{\tau}f\right]_{\tau=\tau_b}J_m-\left[D_m^{\tau\tau}\frac{\partial f}{\partial \tau}+D_m^{\tau j}\frac{\partial f}{\partial u_m^j}-F_m^{\tau}f\right]_{\tau=0}J_m-\frac{\partial \tau_b}{\partial u_m^i}\left[D_m^{i\tau}\frac{\partial f}{\partial \tau}+D_m^{ij}\frac{\partial f}{\partial u_m^j}-F_m^i f\right]_{\tau=\tau_b}J_m+\frac{\partial}{\partial u_m^i}J_m\int_0^{\tau_b}d\tau\left(D_m^{i\tau}\frac{\partial f}{\partial \tau}+D_m^{ij}\frac{\partial f}{\partial u_m^j}-F_m^i f\right)$$

$$+J_m\int_0^{\tau_b} d\tau\left(-\frac{\partial f}{\partial t}-\nu_0 f+Q\right). \tag{41}$$

Equation (41) can be more compactly written introducing the particle flux density Γ_m through the d^4u_m element of the four dimensional (4-D) surface of the Poincaré cut,

$$\Gamma_m \equiv J_m\left[f-D_m^{\tau\tau}\frac{\partial f}{\partial \tau}-D_m^{\tau j}\frac{\partial f}{\partial u_m^j}+F_m^{\tau} f\right]_{\tau=0}, \tag{42}$$

which is just the sum of all contributions from $\tau=0$ in (41).

The Jacobian of variables (34) and (35) expressed through J_m is

$$J_{m'}=J_m\frac{\partial(\tau,\boldsymbol{u}_m)}{\partial(\tau',\boldsymbol{u}_{m'})}=J_m\frac{\partial(\boldsymbol{u}_m)}{\partial(\boldsymbol{u}_{m'})}. \tag{43}$$

The distribution function transforms as a scalar ($f'=f$ for the same physical point), while the diffusion flux density transforms as a contravariant vector,

$$\begin{aligned}
&F_{m'}^{\tau'}f'-D_{m'}^{\tau'\tau'}\frac{\partial f'}{\partial \tau'}-D_{m'}^{\tau' i}\frac{\partial f'}{\partial u_{m'}^i}\\
&\quad=F_m^{\tau}f-D_m^{\tau\tau}\frac{\partial f}{\partial \tau}-D_m^{\tau i}\frac{\partial f}{\partial u_m^i}\\
&\qquad-\frac{\partial \tau_b}{\partial u_m^i}\left(F_m^i f-D_m^{i\tau}\frac{\partial f}{\partial \tau}-D_m^{ij}\frac{\partial f}{\partial u_m^j}\right).
\end{aligned} \tag{44}$$

Therefore, the sum of contributions from $\tau=\tau_b(\boldsymbol{u}_m)$ in (41) is the particle flux density through the cut m' expressed in variables associated with the cut m. As a result, (41) may be cast into the short form

$$\begin{aligned}
&\Gamma_{m'}(t,\boldsymbol{u}_{m'})\frac{\partial(\boldsymbol{u}_{m'})}{\partial(\boldsymbol{u}_m)}-\Gamma_m(t,\boldsymbol{u}_m)\\
&\quad=\frac{\partial}{\partial u_m^i}J_m\int_0^{\tau_b}d\tau\left(D_m^{i\tau}\frac{\partial f}{\partial \tau}+D_m^{ij}\frac{\partial f}{\partial u_m^j}-F_m^i f\right)\\
&\qquad+J_m\int_0^{\tau_b}d\tau\left(-\frac{\partial f}{\partial t}-\nu_0 f+Q\right),
\end{aligned} \tag{45}$$

where $\boldsymbol{u}_{m'}$ is connected to $\boldsymbol{u}_m$ by the mapping (35).

Compared to the bounce time, diffusion processes have a much longer time scale, $\nu_c\tau_b\ll 1$, and the dependence of the distribution function on τ in the right-hand side of (29), respectively (45), can be neglected when moving from one Poincaré cut to the next. By the same order of magnitude, this is also true for the collision terms in the flux density (42), i.e.,

$$\Gamma_m\approx J_m f. \tag{46}$$

Introducing the notation for the quantities integrated along the orbit over one bounce period as

$$\overline{A(\boldsymbol{u}_m)}\equiv\int_0^{\tau_b}d\tau A(\tau,\boldsymbol{u}_m), \tag{47}$$

the following difference-differential equation for the flux density is obtained,

$$\begin{aligned}
&\Gamma_{m'}(t,\boldsymbol{u}_{m'})\frac{\partial(\boldsymbol{u}_{m'})}{\partial(\boldsymbol{u}_m)}\\
&\quad=\Gamma_m(t,\boldsymbol{u}_m)+\frac{\partial^2}{\partial u_m^i\partial u_m^j}\overline{D_m^{ij}}(\boldsymbol{u}_m)\Gamma_m(t,\boldsymbol{u}_m)\\
&\qquad-\frac{\partial}{\partial u_m^i}\mathscr{F}_m^i(\boldsymbol{u}_m)\Gamma_m(t,\boldsymbol{u}_m)-\tau_b(\boldsymbol{u}_m)\frac{\partial}{\partial t}\Gamma_m(t,\boldsymbol{u}_m)\\
&\qquad-\overline{\nu_0}(\boldsymbol{u}_m)\Gamma_m(t,\boldsymbol{u}_m)+\mathscr{Q}(\boldsymbol{u}_m),
\end{aligned} \tag{48}$$

with the variables $\boldsymbol{u}_{m'}$ related to $\boldsymbol{u}_m$ by (35). Here, effective force $\mathscr{F}$ and source $\mathscr{Q}$ are defined as

$$\mathscr{F}_m^i(\boldsymbol{u}_m)=\overline{F_m^i}(\boldsymbol{u}_m)+\frac{1}{J_m}\frac{\partial}{\partial u_m^j}J_m\overline{D_m^{ij}}(\boldsymbol{u}_m), \tag{49}$$

$$\mathscr{Q}=J_m\overline{Q}(\boldsymbol{u}_m). \tag{50}$$

If slow diffusion processes are considered, the continuous time derivative in (48) can be replaced by a finite difference quotient and time can be just considered as an additional mapping variable, $t=t_m$, which transforms as

$$t_{m'}=t_m+\tau_b(\boldsymbol{u}_m). \tag{51}$$

Finally, (48) can be cast into operator form,

$$\Gamma=\hat{M}\Gamma+S_T, \tag{52}$$

where, neglecting terms quadratic in $\nu_c\tau_b$,

$$\hat{M}=\hat{M}^{(L)}\hat{M}^{(T)}\hat{M}^{(D)}(1-\overline{\nu_0}). \tag{53}$$

The integral operator $\hat{M}^{(L)}$ describes the unperturbed mapping in phase space,

$$\begin{aligned}
\hat{M}^{(L)}\Gamma_m(t_{m'},\boldsymbol{u}_m)&=\Gamma_{m'}(t_{m'},\boldsymbol{u}_{m'})\\
&\equiv\sum_{m=m'-1,m',m'+1}\int d^4u_m\\
&\quad\times M^{(L)}(\boldsymbol{u}_{m'},\boldsymbol{u}_m)\Gamma_m(t_{m'},\boldsymbol{u}_m).
\end{aligned} \tag{54}$$

The kernel $M^{(L)}$ is

$$M^{(L)}(\boldsymbol{u}_{m'},\boldsymbol{u}_m)=\Delta_{m'}(\boldsymbol{u}_m)\,\delta(\boldsymbol{u}_{m'}-\hat{\boldsymbol{U}}_m(\boldsymbol{u}_m)), \tag{55}$$

with $\hat{U}_m$ given by (35). The quantity Δ formally defines the groups of particles with respect to the mapping

$$\Delta_{m'}=\begin{cases}\delta_{m',m+1}, & \text{for co-passing,}\\ \delta_{m',m-1}, & \text{for counter-passing,}\\ \delta_{m',m}, & \text{for trapped.}\end{cases} \tag{56}$$

The integral operator $\hat{M}^{(T)}$ describes the time shift during the mapping,

$$\begin{aligned}
\hat{M}^{(T)}\Gamma_m(t_m,\boldsymbol{u}_m)&=\Gamma_m(t_{m'},\boldsymbol{u}_m)\\
&\equiv\int_0^{T-\tau_b(\boldsymbol{u}_m)}dt_m\,\delta(t_{m'}-t_m-\tau_b(\boldsymbol{u}_m))\\
&\quad\times\Gamma_m(t_m,\boldsymbol{u}_m).
\end{aligned} \tag{57}$$

The differential operator $\hat{M}^{(D)}$ describes the diffusion during the mapping,

$$\hat{M}^{(D)}\Gamma_m(t_m,\boldsymbol{u}_m)$$
$$=\Gamma_m(t_m,\boldsymbol{u}_m)+\frac{\partial^2}{\partial u_m^i \partial u_m^j}\overline{D_m^{ij}}(\boldsymbol{u}_m)\Gamma_m(t_m,\boldsymbol{u}_m)$$
$$-\frac{\partial}{\partial u_m^i}\mathscr{F}_m^i(\boldsymbol{u}_m)\Gamma_m(t_m,\boldsymbol{u}_m). \tag{58}$$

The general source term S_T covers the initial conditions with respect to time and possible sources in phase space,

$$S_T=\Gamma_{m'}^{(0)}(\boldsymbol{u}_{m'})H(\tau_b(\boldsymbol{u}_{m'})-t_{m'})+\hat{M}^{(L)}\hat{M}^{(T)}\mathscr{Q}, \tag{59}$$

where H represents the Heaviside step function and $\Gamma_{m'}^{(0)}(\boldsymbol{u}_{m'})$ is the initial value of flux in time.

If one is interested in finding the stationary distribution, the corresponding operator form can be obtained by setting the time derivative of Γ_m in (48) to zero,

$$\Gamma=\hat{M}_s\Gamma+S_s, \tag{60}$$

where

$$\hat{M}_s=\hat{M}^{(L)}\hat{M}^{(D)}(1-\overline{\nu_0}), \quad S_s=\hat{M}^{(L)}\mathscr{Q}. \tag{61}$$

III. MONTE CARLO ALGORITHM

Generally speaking, both (52) and (60) are second kind integral equations and can be solved with appropriate methods. In particular, these types of equations have been successfully solved with Monte Carlo methods by averaging over Markov chains.[24] Actually, the operators $\hat{M}$ and $\hat{M}_s$ define stochastic mappings with transition probability densities given by the kernels of the integral operators $M^{(L)}$, $M^{(T)}$, and $M^{(D)}$ which can be also represented in integral form,

$$\hat{M}^{(D)}\Gamma_m(t,\boldsymbol{u}_m)$$
$$=\int d^4u_{m'}\left(\delta(\boldsymbol{u}_m-\boldsymbol{u}_{m'})+\overline{D_m^{ij}}\frac{\partial^2\delta(\boldsymbol{u}_m-\boldsymbol{u}_{m'})}{\partial u_m^i\partial u_m^j}\right.$$
$$\left.-\mathscr{F}_m^i\frac{\partial\delta(\boldsymbol{u}_m-\boldsymbol{u}_{m'})}{\partial u_m^i}\right)\Gamma_m(t,\boldsymbol{u}_{m'}). \tag{62}$$

This type of integral kernel can be approximated by

$$(\cdots)=\langle\delta(\boldsymbol{u}_m-\boldsymbol{u}_{m'}-\delta\boldsymbol{u}_m(\boldsymbol{u}_{m'}))\rangle, \tag{63}$$

where $\delta\boldsymbol{u}_m(\boldsymbol{u}_{m'})$ is a stochastic process and $\langle\cdots\rangle$ denotes ensemble averaging. The expression in the brackets in (63) is the formal expansion of the δ function in a Taylor series over δu_m^i up to second order if the δu_m^i satisfy the relations

$$\langle\delta u_m^i\rangle=\mathscr{F}_m^i(\boldsymbol{u}_m),$$
$$\langle\delta u_m^i\delta u_m^j\rangle=2\overline{D_m^{ij}}(\boldsymbol{u}_m). \tag{64}$$

It should be noted that this expansion is formal and in order to check for the significance of higher-order terms one has to estimate the derivatives of Γ_m, $\overline{D_m}$, and $\overline{F_m}$, rather than those of the δ function. Within the present approximation of weak collisions it is $|\overline{D_m^{ij}}|\sim|u^iu^j|\tau_b/\tau_{\rm coll}\ll|u^iu^j|$, $|\overline{F_m^i}|\sim|u^i|\tau_b/\tau_{\rm coll}\ll|u^i|$, and therefore the contributions of the higher-order moments in the expansion are already quadratic in $\tau_b/\tau_{\rm coll}$ and can be neglected (derivatives are estimated as $|\partial\Gamma/\partial u_m|\approx\Gamma/u_m$).

With the use of (63) Markov chains (stochastic trajectories) can be constructed according to the following algorithm:

(i) particles are removed from the cuts with the probability equal to $\overline{\nu_0}(\boldsymbol{u}_m)$;
(ii) the remaining particles are shifted in u_m^i by δu_m^i on the cut with the averages of random shift δu_m^i satisfying (64); for the particular way of constructing δu_m^i see, e.g., Refs. 6 and 7;
(iii) new particles are added to the cuts with local probability density $\mathscr{Q}(\boldsymbol{u}_m)$;
(iv) all particles are moved from cut m to the new cut m' according to (35) and (51).

Such an algorithm would be already somewhat faster than the direct Monte Carlo method, because it demands only one Monte Carlo step per bounce time instead of per each trajectory integration step. On the other hand, the method is still less efficient than methods using bounce (canonical) averaging because the number of random steps per collision time is defined by the number of mappings (particle passes through the cuts) during a collision time and this number can be very large. However, in Section V it will be shown how the method can be generalized to construct a much more effective algorithm based on multiple passes.

IV. COMPUTATION OF DIFFUSION COEFFICIENTS

The central point of the method proposed in the present paper is the separation of finding the diffusion coefficients (47) as a pure dynamical problem from the statistical problem needed to solve the full kinetic equation. As will be shown below in this section, for the costly determination of the diffusion coefficients, available integration algorithms for the equations of motions of the ''direct'' MC methods can be used if the random steps are switched off.

The mapping transform (35) and (51) is numerically realized by integrating a mesh of initial values $\boldsymbol{u}_m$ on the Poincaré cut m up to the cut m'. Together with the trajectory, an additional set of equations outlined below has to be integrated in order to obtain friction force, diffusion tensor, and source. Finally, the mapping transform function (35), the diffusion tensor (47) with (30), the effective friction force (49), and source (50) at any point within the cut are obtained by interpolation over the mesh grid.

The integrals of the effective source $\overline{Q}$ and sink probability $\overline{\nu_0}$ along the trajectories are found by solving the additional differential equations

$$\frac{\partial}{\partial\tau}\overline{Q}=Q, \quad \overline{Q}_{\tau=0}=0,$$
$$\frac{\partial}{\partial\tau}\overline{\nu_0}=\nu_0, \quad \overline{\nu_0}|_{\tau=0}=0. \tag{65}$$

The diffusion coefficients $\overline{D_m}$ and friction force $\overline{F_m}$ are obtained in the same way as solutions of additional differential equations

$$\frac{\partial}{\partial \tau}\overline{D_m^{ij}} = D_m^{ij}, \quad \overline{D_m^{ij}}|_{\tau=0} = 0,$$
$$\frac{\partial}{\partial \tau}\overline{F_m^{i}} = F_m^{i}, \quad \overline{F_m^{i}}|_{\tau=0} = 0. \tag{66}$$

The right-hand sides of (66) contain the tensor products of the given diffusion coefficients D^{ij} and friction force F^i with the transformation matrix $\overline{c}^{\,i}_{\,k}$ according to (30). The transformation matrix $\overline{c}^{\,i}_{\,k}$ defined in (32) is the inverse to c_i^k defined as

$$c_i^k = \frac{\partial z^k}{\partial \tau}, \quad i:\tau,$$
$$c_i^k = \frac{\partial z^k}{\partial u_m^i}, \quad i:u_m^i. \tag{67}$$

The equations for the coefficients c_i^k are obtained by differentiating the trajectory equations (19) with respect to u_m^i. The resulting set of equations can be cast into matrix form,

$$\frac{\partial}{\partial \tau} c_i^k = T_j^k c_i^j, \tag{68}$$

where the matrix T_j^k is the Jacobian matrix of the generalized velocity field given by

$$T_j^k = \frac{\partial V^k}{\partial z^j} = \begin{Vmatrix} \dfrac{\partial \Omega}{\partial \vartheta} & \dfrac{\partial \Omega}{\partial u^j} \\ \dfrac{\partial w^k}{\partial \vartheta} & \dfrac{\partial w^k}{\partial u^j} \end{Vmatrix}. \tag{69}$$

The initial conditions follow from (19) for small τ,

$$c_j^i|_{\tau=0} = \begin{Vmatrix} \Omega(\vartheta_{(m)}(\boldsymbol{u}_m), \boldsymbol{u}_m) & \dfrac{\partial \vartheta_{(m)}(\boldsymbol{u}_m)}{\partial u_m^j} \\ w^i(\vartheta_{(m)}(\boldsymbol{u}_m), \boldsymbol{u}_m) & \delta_j^i \end{Vmatrix}. \tag{70}$$

Using the identity

$$\frac{\partial}{\partial \tau}\delta^{\,i}_{\,j} = \frac{\partial}{\partial \tau} c_k^i \overline{c}^{\,k}_{\,j} = 0, \tag{71}$$

the equation for the required coefficients $\overline{c}^{\,i}_{\,j}$ is obtained from (68),

$$\frac{\partial}{\partial \tau}\overline{c}^{\,i}_{\,j} = -\overline{c}^{\,i}_{\,k} T_j^k. \tag{72}$$

The appropriate set of initial conditions follows from the inversion of (70),

$$(\overline{c}^{\,i}_{\,j})_{\tau=0} = \frac{1}{\Omega - w^k \dfrac{\partial \vartheta_{(m)}}{\partial u_m^k}} \times \begin{Vmatrix} 1 & -\dfrac{\partial \vartheta_{(m)}}{\partial u_m^j} \\ -w^i & \left(\Omega - w^k \dfrac{\partial \vartheta_{(m)}}{\partial u_m^k}\right)\delta^{\,i}_{\,j} + w^i \dfrac{\partial \vartheta_{(m)}}{\partial u_m^j} \end{Vmatrix}, \tag{73}$$

where all functions of phase space coordinates have to be evaluated at $u^i = u_m^i$ and $\vartheta = \vartheta_{(m)}(\boldsymbol{u}_m)$.

The solution of the additional equations (65), (66), and (72) provide the complete set of functions needed in the statistical problem formulated in (48). Note that the coefficients $\overline{c}^{\,i}_{\,j}$ are not needed for the solution of the problem and therefore only 20 equations out of the whole set in (72) have to be actually solved. Taking into account the symmetry of the diffusion tensor, the total number of additional equations, even in the general case, can be reduced to 36.

In specific applications, the number of the additional equations can often be further reduced. For example, such a reduction is possible if the initial kinetic equation (1) does not contain the effects of the anomalous diffusion and if the neoclassical diffusion resulting from the collision modified drift motion on time scales of the order of the bounce time is not of interest for the particular problem. In this case, when deriving the Jacobian matrix (69), the particle motion should be considered just as a motion along magnetic field lines with parallel velocity $v_\parallel$,

$$v^i = \frac{v_\parallel}{B}\boldsymbol{B}\cdot\nabla x^i, \quad i = 1,\ldots,3. \tag{74}$$

Then it follows from (72) that (x and y are space and momentum space coordinates)

$$\overline{c}^{\,i}_{\,j} = 0, \quad \text{for } i:x_m^i, \quad j:y^j, \tag{75}$$

because for any function $g(\boldsymbol{z})$ the following identity is valid

$$\begin{aligned} \frac{\partial}{\partial \tau}\left(\frac{\partial u_m^i}{\partial z^k}\right) &= -\frac{\partial u_m^i}{\partial z^l}\left(g\frac{\partial}{\partial z^k}\frac{V^l}{g} + \frac{V^l}{g}\frac{\partial g}{\partial z^k}\right) \\ &= -\left(\frac{\partial u_m^i}{\partial z^l} g \frac{\partial}{\partial z^k}\frac{V^l}{g} + \frac{\partial \ln(g)}{\partial z^k}\frac{\partial u_m^i}{\partial \tau}\right) \\ &= -\frac{\partial u_m^i}{\partial z^l} g \frac{\partial}{\partial z^k}\frac{V^l}{g}, \end{aligned} \tag{76}$$

where the independence of u_m^i on τ has been used. Using this identity with $g = v_\parallel$ and (74) in (69) for finding $\underline{\boldsymbol{T}}$, (75) immediately follows. Therefore, diffusion tensor D_m^{ij} and force $\overline{F_m^i}$ have zero components with respect to the spatial variables x_m^i (no ''short scale'' neoclassical transport).

The rest of transformation coefficients (actually still four of them, $\overline{c}^{\,i}_{\,j}, i:y_m, j:y$, are needed) can be obtained by direct solution of (72). However, this can be done in a shorter way if use is made of conservation of energy E and magnetic moment μ,

$$E = m_0 c^2 \gamma + e\varphi, \quad \mu = \frac{p^2(1-\lambda^2)}{2m_0 B}, \tag{77}$$

where γ is given by (6). From this it follows immediately,

$$\frac{\partial p_m}{\partial p} = \frac{p\,\gamma_m}{p_m \gamma}, \quad \frac{\partial p_m}{\partial \lambda} = 0,$$
$$\frac{\partial \lambda_m}{\partial p} = \frac{1-\lambda_m^2}{p^2 \lambda_m}\left(\frac{p^3 \gamma_m}{p_m^3 \gamma} - 1\right), \quad \frac{\partial \lambda_m}{\partial \lambda} = \frac{\lambda(1-\lambda_m^2)}{\lambda_m(1-\lambda^2)}, \tag{78}$$

where γ_m is the relativistic factor on the minimum surface $\boldsymbol{u} = \boldsymbol{u}_m$.

In the considered case, the number of additional equations to be integrated together with the particle orbits has been reduced to seven. As the drift motion is retained in the trajectories but neglected in the transformation matrix, the model will still cover direct orbit losses of trapped particles occurring in systems without toroidal symmetry.

V. MULTIPASS METHOD

So far, the difference in time scales between bounce time τ_b and collision time τ_c has been used to neglect the effect of collisions when integrating the collision tensor etc. over a bounce time along the orbit. Collisions can then be taken into account each mapping procedure (single-pass method). This is already more advantageous than the direct Monte Carlo procedure where this is done each Runge–Kutta integration step. Nevertheless, such a single-pass procedure will not remove the stiffness of the problem inherent in the different time scales. If the evolution of the distribution function is to be modeled during one collision time and collisions are rare, several hundred thousands of mappings may be needed to obtain reliable results.

In order to save computer time it is desirable to perform n mappings at once before doing a Monte Carlo step. The number n should be in the range $1 \ll n \ll \tau_c/\tau_b$. In this case, n can be chosen in such a way that a required accuracy ε with respect to the systematic error in modeling diffusion can be achieved if $n = \varepsilon \tau_c/\tau_b$. The number of actual Monte Carlo steps N_{MC} per one collision time is then defined by the accuracy parameter ε, $N_{\mathrm{MC}} = 1/\varepsilon$ instead of system collisionality and thus provides a solution to the stiffness problem.

The multipass equation is derived analogous to the single-pass equation but with the replacement of the single-pass bounce time $\tau_b(\boldsymbol{u}_m)$ by the n-pass bounce time $\tau_b^{(n)}(\boldsymbol{u}_{m_0})$ defined as the time required the particle needs to reach a certain cut after n mappings starting from $\boldsymbol{u}_{m_0}$ in the cut m_0. It can be written as a sum of single-pass bounce times,

$$\tau_b^{(n)}(\boldsymbol{u}_{m_0}) = \tau_b(\boldsymbol{u}_{m_0}) + \tau_b(\boldsymbol{u}_{m_1}) + \cdots + \tau_b(\boldsymbol{u}_{m_{n-1}}). \tag{79}$$

The vector $\boldsymbol{u}_{m_k}$ is the particle position after k mappings,

$$\begin{aligned} u^i_{m_k} &= \hat{U}^i_{m_k}(\boldsymbol{u}_{m_0}) \\ &\equiv \hat{U}^i(\tau_b^{(k)}(\boldsymbol{u}_{m_0}), \boldsymbol{u}_{m_0}) \\ &= \hat{U}^i(\tau_b(\boldsymbol{u}_{m_{k-1}}) + \tau_b^{(k-1)}(\boldsymbol{u}_{m_0}), \boldsymbol{u}_{m_0}) \\ &= \hat{U}^i(\tau_b(\boldsymbol{u}_{m_{k-1}}), \hat{U}^i(\tau_b^{(k-1)}(\boldsymbol{u}_{m_0}), \boldsymbol{u}_{m_0})) \\ &= \hat{U}^i(\tau_b(\boldsymbol{u}_{m_{k-1}}), \boldsymbol{u}_{m_{k-1}}). \end{aligned} \tag{80}$$

Here, the group property of the orbits (17) has been used. If the bounce time is redefined in this way, (47) and (48) can still be used in their present form.

The multipass value of any trajectory integrated vector function, e.g., $\overline{F^{(n)i}}(\boldsymbol{u}_{m_0})$, can be composed from its respective single-pass values in the following way,

$$\begin{aligned} \overline{F^{(n)i}}(\boldsymbol{u}_{m_0}) &= \int_0^{\tau_b^{(n)}(\boldsymbol{u}_{m_0})} d\tau \frac{\partial u^i_{m_0}}{\partial z^\alpha} F^\alpha \Bigg|_{\vartheta = \hat{\Theta}(\tau, \boldsymbol{u}_{m_0}), \boldsymbol{u} = \hat{\boldsymbol{u}}(\tau, \boldsymbol{u}_{m_0})} \\ &= \left(\int_0^{\tau_b(\boldsymbol{u}_{m_0})} d\tau + \int_0^{\tau_b(\boldsymbol{u}_{m_1})} d(\tau - \tau_b(\boldsymbol{u}_{m_0})) + \cdots + \int_0^{\tau_b(\boldsymbol{u}_{m_{n-1}})} d(\tau - \tau_b^{(n-1)}(\boldsymbol{u}_{m_0})) \right)(\cdots) \\ &= \int_0^{\tau_b(\boldsymbol{u}_{m_0})} d\tau \frac{\partial u^i_{m_0}}{\partial z^\alpha} F^\alpha \Bigg|_{\vartheta = \hat{\Theta}(\tau, \boldsymbol{u}_{m_1}), \boldsymbol{u} = \hat{\boldsymbol{u}}(\tau, \boldsymbol{u} m_1)} + \cdots + \int_0^{\tau_b(\boldsymbol{u}_{m_{n-1}})} d\tau \frac{\partial u^i_{m_0}}{\partial z^\alpha} F^\alpha \Bigg|_{\vartheta = \hat{\Theta}(\tau, \boldsymbol{u}_{m_{n-1}}), \boldsymbol{u} = \hat{U}(\tau, \boldsymbol{u}_{m_{n-1}})} \\ &= \overline{F^i_m}(\boldsymbol{u}_{m_0}) + \frac{\partial u^i_{m_0}}{\partial u^\alpha_{m_1}} \overline{F^\alpha_{m_1}}(\boldsymbol{u}_{m_1}) + \cdots + \frac{\partial u^i_{m_0}}{\partial u^{\alpha_1}_{m_1}} \frac{\partial u^{\alpha_1}_{m_1}}{\partial u^{\alpha_2}_{m_2}} \cdots \frac{\partial u^{\alpha_{n-2}}_{m_{n-2}}}{\partial u^{\alpha_{n-1}}_{m_{n-1}}} \overline{F^{\alpha_{n-1}}_{m_{n-1}}}(\boldsymbol{u}_{m_{n-1}}). \end{aligned} \tag{81}$$

Here, the vector transformation matrices from cut m_k to cut m_{k+1} are the values of the respective functions $\overline{c}^i_j$ (32) evaluated at the bounce time $\tau_b(\boldsymbol{u}_{m_k})$,

$$\frac{\partial u^i_{m_k}}{\partial u^j_{m_{k+1}}} = \overline{c}^i_j(\vartheta,\boldsymbol{u})\big|_{\vartheta=\hat{\Theta}(\tau_b(\boldsymbol{u}_{m_k}),\boldsymbol{u}_{m_k}),\boldsymbol{u}=\hat{\boldsymbol{u}}(\tau_b(\boldsymbol{u}_{m_k}),\boldsymbol{u}_{m_k})}. \tag{82}$$

Expressions for multipass values of scalar (source) and tensor (diffusion) function can be composed from their respective single-pass values in an analogous way.

Therefore, once the single-pass values have been obtained and stored together with the transformation matrices for each map, multipass values can be effectively composed without further numerical effort. In this setup, the Monte Carlo steps can now be introduced in the same way as described in Section III.

VI. GLOBAL VALUES AND AVERAGED MOMENTS

In this section it is shown how to compute global values of any function, say $\mathscr{A}$, of dynamical variables defined by

$$\langle\mathscr{A}\rangle = \int d^6z J f \mathscr{A} = 2\pi \int d^4u \int d\vartheta J f \langle\mathscr{A}\rangle_\phi, \tag{83}$$

where the Jacobian J and the distribution function f are assumed to be independent of gyrophase ϕ and $\langle\mathscr{A}\rangle_\phi$ is the average of $\mathscr{A}$ with respect to ϕ

$$\langle\mathscr{A}\rangle_\phi = \frac{1}{2\pi}\int_0^{2\pi} d\phi \mathscr{A}. \tag{84}$$

The phase space is first separated by Poincaré cuts numbered by m. On each Poincaré cut, the free particle orbits are introduced as local Lagrangian variables. After a finite ''bounce'' time τ_b, these orbits will hit either the nearest next Poincaré cut $m\pm1$ (passing orbits) or again the cut m itself (trapped orbits). In order to make the transformation to the local coordinate system unique, the phase space has to be divided into regions such that in each region the trapped orbits belong to a single cut (see Fig. 2). In Eulerian variables, the global value can then be written as

$$\begin{aligned}\langle\mathscr{A}\rangle = 2\pi\Bigg(&\int_{\text{trapped}} d^4u \sum_m \int_{\vartheta_{(m-\frac{1}{2})}(\boldsymbol{u})}^{\vartheta_{(m+\frac{1}{2})}(\boldsymbol{u})} d\vartheta \\ &+ \int_{\text{co-passing}} d^4u \sum_m \int_{\vartheta_{(m)}(\boldsymbol{u})}^{\vartheta_{(m+1)}(\boldsymbol{u})} d\vartheta \\ &+ \int_{\text{counter-passing}} d^4u \sum_m \int_{\vartheta_{(m-1)}(\boldsymbol{u})}^{\vartheta_{(m)}(\boldsymbol{u})} d\vartheta \Bigg) |J| f \langle\mathscr{A}\rangle_\phi.\end{aligned} \tag{85}$$

The phase space is traced out by the orbits completely and in local variables $(\tau,\boldsymbol{u}_m)$ the global value becomes

$$\langle\mathscr{A}\rangle = 2\pi\sum_m \int d^4u_m \int_0^{\tau_b(\boldsymbol{u}_m)} d\tau |J_m| f \langle\mathscr{A}\rangle_\phi. \tag{86}$$

From (14), J_m is independent of τ and, in lowest order in bounce over collision time, this is also true for the distribution function f. Therefore, both can be taken out of the integration over τ. Together with the notation for the flux density $\Gamma_m = J_m f$, the global value simply becomes

$$\langle\mathscr{A}\rangle = 2\pi\sum_m \int d^4u_m |\Gamma_m(\boldsymbol{u}_m)| \overline{\langle\mathscr{A}\rangle}_\phi, \tag{87}$$

where $\overline{\langle\mathscr{A}\rangle}_\phi$ is the trajectory integrated function defined in (47). As an example, the total number of particles in the system is obtained by setting $\mathscr{A}=1$, and therefore

$$N = 2\pi\sum_m \int d^4u_m |\Gamma_m(\boldsymbol{u}_m)| \tau_b(\boldsymbol{u}_m). \tag{88}$$

Also, taking into account electrostatic fields the total energy $\mathscr{E} = \gamma mc^2 + e\phi$ is conserved along the orbit and therefore

$$\langle\mathscr{E}\rangle = 2\pi\sum_m \int d^4u_m |\Gamma_m(\boldsymbol{u}_m)| \tau_b(\boldsymbol{u}_m) \mathscr{E}(\boldsymbol{u}_m). \tag{89}$$

The evolution of the global values defined above is obtained by multiplying (48) by $\text{sgn}(J_m)\langle\mathscr{A}\rangle_{bm}$, where $\langle\mathscr{A}\rangle_{bm} \equiv \overline{\langle\mathscr{A}\rangle}_\phi(\boldsymbol{u}_m)/\tau_b(\boldsymbol{u}_m)$, then integrating over d^4u_m, and, finally, summation over m,

$$\begin{aligned}\frac{\partial}{\partial t}\langle\mathscr{A}\rangle = 2\pi\sum_m \int d^4u_m\ \text{sgn}(J_m) \\ \times\langle\mathscr{A}\rangle_{bm}\Bigg\{ \frac{\partial^2}{\partial u^i_m \partial u^j_m} \overline{D^{ij}_m}(\boldsymbol{u}_m)\Gamma_m(t,\boldsymbol{u}_m) - \frac{\partial}{\partial u^i_m} \\ \times \mathscr{F}^i_m(\boldsymbol{u}_m)\Gamma_m(t,\boldsymbol{u}_m) - \overline{\nu_0}(\boldsymbol{u}_m)\Gamma_m(t,\boldsymbol{u}_m) \\ + \mathscr{Q}(\boldsymbol{u}_m)\Bigg\} + 2\pi\sum_m \int d^4u_m |\Gamma_m(t,\boldsymbol{u}_m)| \big(\langle\mathscr{A}\rangle_{bm} \\ - \langle\mathscr{A}\rangle_{bm'}\big),\end{aligned} \tag{90}$$

where $m' = m-1,\ m+1,\ m$ for copassing, counterpassing, and trapped orbits, respectively. If $\langle\mathscr{A}\rangle_\phi$ is an invariant of motion, then it is independent on τ, so that $\langle\mathscr{A}\rangle_{bm} = \langle\mathscr{A}\rangle_\phi$. In this case, the last term in (90) cancels. For example, the evolution of the total energy discussed above is

$$\begin{aligned}\frac{\partial}{\partial t}\mathscr{E} = 2\pi\sum_m \int d^4u_m \Bigg\{ |\Gamma_m(t,\boldsymbol{u}_m)| \Bigg(\frac{\overline{D^{pp}_m}}{m\gamma^3} + \frac{p_m}{m\gamma}\overline{F^p_m} \\ - \overline{\nu_0}\mathscr{E} + \text{sgn}(J_m)\mathscr{Q}\mathscr{E}\Bigg)\Bigg\}.\end{aligned} \tag{91}$$

This formula is useful to compute the power deposition inside the system due to auxiliary heating.

VII. BOUNCE AVERAGING

In certain cases the stochastic mapping equation (48) can be simplified to differential form. For example, this can always be done in phase space regions of strictly trapped particles as a result of the smallness of the gyroradius compared to the system nonuniformity scale, and the smallness of the drift velocity compared to the parallel one, respectively.

Assuming $\boldsymbol{u}_{m'} \approx \boldsymbol{u}$ and taking into account (46) and (43) the left-hand side of the double-pass mapping equation (48) is expanded up to linear order with respect to the small difference $u^i_{m'} - u^i_m$,

$$\frac{\partial f}{\partial t} + \langle w^i \rangle^{(2)}_b \frac{\partial f}{\partial u^i_m} = \frac{1}{\tau^{(2)}_b J_m} \frac{\partial}{\partial u^i_m} \tau^{(2)}_b J_m \left(\langle D^{ij}_m \rangle^{(2)}_b \frac{\partial f}{\partial u^j_m} - \langle F^i_m \rangle^{(2)}_b f \right) - \langle \nu_0 \rangle^{(2)}_b f + \langle Q \rangle^{(2)}_b , \tag{92}$$

where $\tau^{(2)}_b$ is the double-pass bounce time (79) and the n-pass bounce averages have been defined as [see also (81)],

$$\langle A_m \rangle^{(n)}_b = \frac{1}{\tau^{(n)}_b} \overline{A^{(n)}} = \frac{1}{\tau^{(n)}_b} \int_0^{\tau^{(n)}_b} d\tau A_m . \tag{93}$$

The equations of motion (16) for this limit and the definition (93) give the relation

$$(u^i_{m'} - u^i_m)/\tau^{(2)}_b = \langle w^i \rangle^{(2)}_b , \tag{94}$$

which has been used in (92).

If the momentum space variables are chosen as $\boldsymbol{y} = (E, \mu, \phi)$, where E and μ are the integrals of motion (77), the momentum space components of the velocity (94) vanish, whereas the spatial components can be expressed through the parallel adiabatic invariant

$$J_\parallel = J_\parallel(\boldsymbol{u}_m) = \oint ds \, \gamma v_\parallel , \tag{95}$$

with $\boldsymbol{u}_m = (x^1_m, x^2_m, E, \mu)$ and the integration has to be taken along the trapped orbit which in zero order with respect to drift velocity coincides with the magnetic field line. The spatial components of the averaged velocity are given by

$$\langle w^i \rangle^{(2)}_b = \frac{dx^i_m}{dt} = \frac{1}{\tau^{(2)}_b} \frac{dx^i_m}{dn}, \quad i = 1,2, \tag{96}$$

where the coordinate change per one full (double) bounce period is (see Appendix B),

$$\frac{dx^1_m}{dn} = \frac{m_0 c}{e|J_m|} \frac{\partial J_\parallel}{\partial x^2_m}, \quad \frac{dx^2_m}{dn} = -\frac{m_0 c}{e|J_m|} \frac{\partial J_\parallel}{\partial x^1_m}. \tag{97}$$

In this form, the averaged equations of motion can also be used for the construction of multipass mapping functions. This will be shown for the case when the ''short-scale'' neoclassical transport resulting from the modification by collisions of the trapped trajectory during one bounce period can be neglected. This approximation makes sense for particles which deviate after many bounces significantly, as compared to a single bounce orbit, from the magnetic surface, like ''superbanana'' particles in stellarators. In this case only the momentum-space diffusion coefficients have to be retained in (48) (see Section IV). Due to the invariance of the momentum space variables E and μ, the transformation [matrices (82) reduce to Kronecker symbols],

$$\frac{\partial u^i_{m_k}}{\partial u^j_{m_{k+1}}} = \delta^i_j , \tag{98}$$

where $i,j = 3,4$. The n-pass mapping functions (80) for even $n = 2k$ values are obtained by integrating equations (97) with the time-like variable n changing from 0 to k. The n-pass ''bounce'' time $\tau^{(n)}_b$ (79) and the components of the diffusion term $\overline{D^{(n)ij}}$, $\overline{F^{(n)i}}$, $\overline{\nu^{(n)}}$, and $\overline{Q^{(n)}}$ are then obtained by integrating simultaneously the corresponding double-pass quantities,

$$\overline{A^{(2k)}} = \int_0^k dn \overline{A^{(2)}}. \tag{99}$$

Note that up to now no restrictions have been imposed on the symmetry properties of the trap magnetic field. For systems with rotational symmetry (tokamaks, axially symmetric mirrors) the mapping equation (48) reproduces the result of canonical (bounce) averaging. Without loss of generality, this is shown for the case of a tokamak. In order to obtain the bounce averaged equation, one should place the Poincaré cut in such a way that it also stays symmetric with respect to rotations around the symmetry axis. The midplane obviously satisfies this condition. In this case, one mapping variable which corresponds to the rotation angle with respect to the symmetry axis ($x^2_m = \zeta$–toroidal angle) becomes the cyclic variable of the unperturbed mapping equation (35) in the sense that all mapping functions except $\hat{U}^2_m$ are independent on x^2_m while $\hat{U}^2_m$ is a linear function of x^2_m [see (37)]. Moreover, the rest of the variables remain unchanged with respect to the unperturbed mapping [double-pass mapping for trapped particles, see (36)–(40)] and the bounce time τ_b is also independent on ζ_m.

To start with, the simplest case is considered when local diffusion operators, sources, and sinks are all toroidally symmetric. In this case, the solution to (48) should be looked for in the form independent on the cyclic variable $x^2_m = \zeta$. For such a system, the difference $\Gamma_{m'} [\partial(\boldsymbol{u}_{m'})/\partial(\boldsymbol{u}_m)] - \Gamma_m$ exactly vanishes in (48) for passing particles. Dividing the resulting equation by τ_b, the bounce averaged equation is obtained,

$$\frac{\partial f}{\partial t} = \frac{1}{\tau_b J_m} \frac{\partial}{\partial u^i_m} \tau_b J_m \left(\langle D^{ij}_m \rangle_b \frac{\partial f}{\partial u^j_m} - \langle F^i_m \rangle_b f \right) - \langle \nu_0 \rangle_b f + \langle Q \rangle_b . \tag{100}$$

Here, superscript (1) is omitted for single-pass bounce averages (93). For trapped particles the result is formally the same if one starts from the double-pass equation (48). The only change is the redefinition of τ_b and the bounce-averages to double-pass ones in (100). This result also follows from the more approximate equation (92), in which the term containing the averaged drift velocity vanishes due to the assumed toroidal symmetry.

In order to derive the bounce-averaged equation in the case when local diffusion operators and sources or sinks are toroidally asymmetric, the ansatz introduced in Ref. 25 is used. The collisions are assumed weak enough so that one can use n-pass mapping, where $n = \varepsilon \tau_c / \tau_b \gg 1$ (see Section V) and $n = 2k$ is an even number. Taking Eq. (48) in multipass form, the flux is assumed again to be toroidally symmetric, so that unperturbed mapping terms will cancel each

other. Dividing the equation by $\tau_b^{(n)} J_m$ the bounce-averaged equation takes the same form as before (100), with the bounce averaged quantities taken in multipass form (93). To verify the assumption of toroidally symmetric distribution, it must be shown that all multipass bounce averages entering the final equation are independent on the toroidal mapping variable $u_m^2 = \zeta_m$ as well. As in Section V, this is first checked for the friction force F_m^i. The corresponding checks for the sources, sinks, and diffusion coefficients then follow immediately. Due to the invariance of all variables except the cyclic ζ_m, Eq. (98) is valid if for the index range of i and j the variable $u_m^2 = \zeta_m$ is excluded. At the same time the components of the friction force (and diffusion tensor) which correspond to ζ_m do not contribute in (100) because they appear only in combination with derivatives of the distribution function and friction force or diffusion tensor, which, in turn, vanish because of the assumed toroidal symmetry. Therefore it follows from (81) taking also into account (37) and (98) that

$$\langle F_m^i \rangle_b^{(n)} = \frac{1}{n\tau_b} \sum_{k=0}^{n-1} \overline{F_m^i}(\zeta_m + (2\pi q\sigma + \Delta\zeta)k). \tag{101}$$

In the case of trapped particles, the bounce time τ_b and the bounce-averages in the right-hand side of (101) have to be taken as double-pass ones. Due to periodicity with respect to ζ_m, $\overline{F_m^i}$ can be presented in form of a Fourier series over the toroidal variable ζ

$$\overline{F_m^i}(\zeta) = \langle \overline{F_m^i} \rangle_\zeta + \sum_{l \neq 0} \phi_l \exp(il\zeta), \tag{102}$$

where

$$\langle \overline{F_m^i} \rangle_\zeta \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} d\zeta \overline{F_m^i}(\zeta). \tag{103}$$

From the formula for the sum of geometrical progression it follows

$$\langle F_m^i \rangle_b^{(n)} = \frac{1}{\tau_b} \langle \overline{F_m^i} \rangle_\zeta + O, \tag{104}$$

where

$$O = \frac{1}{n\tau_b} \sum_{l \neq 0} \phi_l \exp(il\zeta_m) \frac{1 - \exp(iln(2\pi q\sigma + \Delta\zeta))}{1 - \exp(il(2\pi q\sigma + \Delta\zeta))}. \tag{105}$$

Obviously the assumption made is verified if the function O which depends on the toroidal variable ζ_m is negligibly small.

Consider first the passing particles, say co-passing with $\sigma = 1$. If the safety factor q is an irrational number and the small term $\Delta\zeta$ is neglected, the denominator in (105) is estimated to be of order one. Therefore O becomes small with a large n or, in other words, the collision frequency should be much less than the bounce frequency. If q is a rational number, say $q = j/k$ with j and k integers, with a large denominator $k \gg 1$, the main contribution to the sum over the toroidal wave numbers l in (105) originates from the term $l = k$ and is estimated to be of order ϕ_k/τ_b. It is small if the force $\overline{F_m^i}$ is not strongly toroidally localized, i.e., $k \gg \Delta k$, where $1/\Delta k$ is the scale of $\overline{F_m^i}$ over toroidal angle. For trapped particles $\sigma = 0$ and $\Delta\zeta \ll 1$, the long-wave toroidal modes $l \sim 1$ are the most dangerous to invalidate the approximation. Only if $n\Delta\zeta \gg 1$, the contribution from these modes is small. Note that the same condition is true for all particles at rational surfaces with low rationality, because in this case $\Delta\zeta$ cannot be neglected for passing particles. On the other hand, this condition can be formulated such that the toroidal rotation time of the bananas should be much less than the collision time,

$$\tau_b / \Delta\zeta \ll \tau_c. \tag{106}$$

If this condition is met, the bounce-averaged equation (100) is shown to be valid even for the case of toroidally asymmetric diffusion operators, sources and sinks. The corresponding bounce-averaged quantities appearing in the final equation are in full agreement with (104), where the small quantity O can be neglected.

Condition (106) is much more restrictive than the condition of a ''collisionless'' confinement limit, $\tau_b \ll \tau_c$, and can be easily violated. In this case the toroidally localized perturbation of the distribution function, e.g., the cyclotron resonance heating with a localized wave packet, may lead to toroidally asymmetric distributions of trapped particles.[26] The effect is even stronger if such heating is performed very near a rational surface[27] where the passing particles also contribute to the toroidal asymmetry. Note that even for a small induced toroidal asymmetry when condition (106) is still valid, the effect of it can cause a significant increase in the cross-field transport through the induced toroidal asymmetry of the ambipolar electric potential.[28] For these cases the Monte Carlo mapping technique based on SME provides an adequate tool to compute the particles distribution function[29] and to study symmetry breaking effects on the cross-field transport.

VIII. CONCLUSION

A stochastic mapping equation has been derived which describes, in the regime of weak collisions, the slow evolution of the particle distribution function in magnetic traps. This equation provides a fairly general discretization of the drift kinetic quasilinear equation with respect to the unperturbed motion.

When canonical (bounce) averaging is applicable, e.g., in magnetic traps with axial space symmetry or phase space regions of trapped particles in asymmetric traps, the corresponding averaged equations are recovered from the stochastic mapping equation.

In contrast to averaging methods, the proposed method never utilizes the integrability condition for the unperturbed particle motion and therefore takes into account in discretized form the variation of the distribution function along the unperturbed trajectories. Thus it is also applicable in the case of generically ''nonintegrable'' motion, e.g., in ergodic magnetic field layers or phase space regions where the particle trajectory is dynamically unstable.

For the solution of the stochastic mapping equation a simple Monte Carlo method is proposed. The mapping tech-

nique introduced allows for a separation of the dynamic motion problem from modeling stochastic processes and thus reduces the required processor time considerably as compared to methods based on the direct modeling of stochastic orbits of test particles.

At the same time, such a separation needs sufficient memory in order to precompute and store the relevant mapping functions. This amount is, however, of the same order which is required by averaging methods if realistic magnetic field configurations are considered. In a number of cases the requirement for computer resources can be reduced by simplifying the spatial transport model and an appropriate choice of independent variables, e.g., using integrals of motion and flux coordinates. There are no restrictions for such a choice, because the whole formalism has been developed for a general set of coordinates and momentum space variables.

The efficiency of the multipass Monte Carlo method proposed in Section V has been tested for a tokamak geometry[29] and turned out to be close to the efficiency of canonically averaged methods.[6]

The proposed method is applicable for modeling transport and heating processes in magnetic traps with broken axial symmetry, such as stellarators or tokamaks with toroidal field ripples, as well as for modeling of kinetic effects in stochastic divertors and other systems with ergodic magnetic field layers, e.g., the Earth's magnetopause, etc.

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APPENDIX A: SURFACE ELEMENT

Let the parametrization of the $n-1$ dimensional surface in any curvilinear coordinate system, say $z^1,z^2,\dots,z^n$ be

$$z^\alpha=\Phi^\alpha(\beta^1,\beta^2,\dots,\beta^{n-1}), \tag{A1}$$

so that the tangential vectors related to the parameters β^i are

$$d\boldsymbol{X}_{\beta^i}=\frac{\partial \boldsymbol{X}}{\partial z^\alpha}\frac{\partial \Phi^\alpha}{\partial \beta^i}d\beta^i \text{ (no summation over } i). \tag{A2}$$

In Cartesian coordinates the surface element is

$$d\boldsymbol{S}=d\boldsymbol{X}_{\beta^1}\wedge d\boldsymbol{X}_{\beta^2}\wedge\cdots\wedge d\boldsymbol{X}_{\beta^{n-1}}. \tag{A3}$$

With (A2) the surface element can be expressed as

$$d\boldsymbol{S}=\left(\frac{\partial \boldsymbol{X}}{\partial z^{\alpha_1}}\wedge\frac{\partial \boldsymbol{X}}{\partial z^{\alpha_2}}\wedge\cdots\wedge\frac{\partial \boldsymbol{X}}{\partial z^{\alpha_{n-1}}}\right)\times\frac{\partial\Phi^{\alpha_1}}{\partial\beta^1}\frac{\partial\Phi^{\alpha_2}}{\partial\beta^2}\cdots\frac{\partial\Phi^{\alpha_{n-1}}}{\partial\beta^{n-1}}d\beta^1d\beta^2\cdots d\beta^{n-1}. \tag{A4}$$

On the other hand,

$$\left(\frac{\partial \boldsymbol{X}}{\partial z^{\alpha_1}}\wedge\frac{\partial \boldsymbol{X}}{\partial z^{\alpha_2}}\wedge\cdots\wedge\frac{\partial \boldsymbol{X}}{\partial z^{\alpha_{n-1}}}\right)\cdot\boldsymbol{e}_\alpha=J\epsilon_{\alpha\alpha_1\alpha_2\cdots\alpha_{n-1}}, \tag{A5}$$

with co- and contravariant basis vectors defined as

$$\boldsymbol{e}_\alpha=\frac{\partial \boldsymbol{X}}{\partial z^\alpha},\quad \boldsymbol{e}^\alpha=\frac{\partial z^\alpha}{\partial \boldsymbol{X}}. \tag{A6}$$

Contracting (A5) with the contravariant vector $\boldsymbol{e}^\alpha$ and using the result in (A4) leads to

$$d\boldsymbol{S}=J\boldsymbol{e}^\alpha\epsilon_{\alpha\alpha_1\alpha_2\cdots\alpha_{n-1}}\frac{\partial\Phi^{\alpha_1}}{\partial\beta^1}\frac{\partial\Phi^{\alpha_2}}{\partial\beta^2}\cdots\frac{\partial\Phi^{\alpha_{n-1}}}{\partial\beta^{n-1}}\times d\beta^1d\beta^2\cdots d\beta^{n-1}. \tag{A7}$$

Let the equation for the surface in curvilinear coordinates be

$$z^n-F(z^1,z^2,\dots,z^{n-1})=0. \tag{A8}$$

On choosing the parametrization as

$$\Phi^\alpha=\beta^\alpha,\quad \alpha=1,\dots,n-1, \tag{A9}$$

$$\Phi^n=F(\beta^1,\beta^2,\dots,\beta^{n-1}), \tag{A10}$$

it follows

$$\frac{\partial\Phi^\alpha}{\partial\beta^i}=\delta_i^\alpha+\delta_n^\alpha\frac{\partial F}{\partial\beta^i}. \tag{A11}$$

Taking into account the properties of the Levi–Civita symbol many terms vanish,

$$\epsilon_{\alpha\alpha_1\alpha_2\cdots\alpha_{n-1}}\frac{\partial\Phi^{\alpha_1}}{\partial\beta^1}\frac{\partial\Phi^{\alpha_2}}{\partial\beta^2}\cdots\frac{\partial\Phi^{\alpha_{n-1}}}{\partial\beta^{n-1}}=\delta_\alpha^n-\frac{\partial F}{\partial\beta^\alpha}, \tag{A12}$$

and, as a result, the covariant component of the surface element vector is

$$d\boldsymbol{S}\cdot\boldsymbol{e}_\alpha=(dS)_\alpha=J\frac{\partial}{\partial z^\alpha}(z^n-F(z^1,z^2,\cdots,z^{n-1}))\Big|_{z^\alpha=\Phi^\alpha(\beta^1,\beta^2,\dots,\beta^{n-1})}\times d\beta^1d\beta^2\cdots d\beta^{n-1}. \tag{A13}$$

APPENDIX B: AVERAGED DRIFT VELOCITY

Let us introduce the space coordinate set (ξ^1,ξ^2,ξ^3), where

$$\xi^3\equiv\vartheta-\vartheta_{(m)}(\boldsymbol{u}), \tag{B1}$$

so that the surface $\xi^3=0$ defined by the additional constraints $E=\text{const}$ and $\mu=\text{const}$ lies within the Poincaré cut (18). On the cut the coordinates ξ^1 and ξ^2 are defined by $\xi^i=x_m^i$, $i=1,2$ and away from the cut they satisfy

$$\mathbf{h}\cdot\nabla\xi^1=\mathbf{h}\cdot\nabla\xi^2=0. \tag{B2}$$

Here, $\mathbf{h}$ is the unit vector along the magnetic field line. The shift per one full bounce period over ξ^1 and ξ^2 is given in Ref. 23 as

$$\frac{d\xi^1}{dn}=\frac{m_0c}{eB}\sqrt{\frac{g_{33}}{g}}\frac{\partial J_\parallel}{\partial\xi_m^2},\quad \frac{d\xi^2}{dn}=-\frac{m_0c}{eB}\sqrt{\frac{g_{33}}{g}}\frac{\partial J_\parallel}{\partial\xi_m^1}, \tag{B3}$$

where g_{33} is the metric tensor component

$$\sqrt{g_{33}}=\left|\frac{\partial \mathbf{r}}{\partial \xi^3}\right|=\frac{1}{|\mathbf{h}\cdot\nabla\xi^3|}, \tag{B4}$$

and g is the metric determinant

$$g=\det\{g_{ij}\}=\left(\frac{\partial \mathbf{r}}{\partial \xi^1}\wedge\frac{\partial \mathbf{r}}{\partial \xi^2}\cdot\frac{\partial \mathbf{r}}{\partial \xi^3}\right)^2. \tag{B5}$$

Taking into account that $\partial \mathbf{r}/\partial\xi^3$ and $\mathbf{h}$ are parallel, from (B5) one gets

$$\sqrt{\frac{g}{g_{33}}}=\frac{\partial \mathbf{r}}{\partial \xi^1}\wedge\frac{\partial \mathbf{r}}{\partial \xi^2}\cdot\mathbf{h}=\frac{\mathbf{h}\cdot d\mathbf{S}_{(\mathbf{x})}}{dx_m^1 dx_m^2}, \tag{B6}$$

where $d\mathbf{S}_{(\mathbf{x})}$ is the element of the surface $\xi^3=$const and x_m^i are the surface parameters. The spatial components of the Poincaré cut element $d\mathbf{S}$ are given by extension to the momentum space

$$d\mathbf{S}=d\mathbf{S}_{(\mathbf{x})}J_y dE\, d\mu. \tag{B7}$$

Assuming the motion in space to be along the magnetic field lines with parallel velocity $v_\parallel$ and using the invariance of the momentum space variables E and μ one gets from (25)

$$\sqrt{\frac{g}{g_{33}}}=\frac{J_m}{J_y v_\parallel}. \tag{B8}$$

Taking into account $J_y=B/|v_\parallel|$, Eq. (97) follows from (B3) and (B8).

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