A BOUNCE-AVERAGED FOKKER-PLANCK CODE FOR STELLARATOR TRANSPORT

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ABSTRACT

A computer code for solving the bounce-averaged Fokker-Planck equation appropriate to stellarator transport has been developed, and its first applications made. The code is much faster than the bounce-averaged Monte-Carlo codes, which up to now have provided the most efficient numerical means for studying stellarator transport. Moreover, because the connection to analytic kinetic theory of the Fokker-Planck approach is more direct than for the Monte-Carlo approach, a comparison of theory and numerical experiment is now possible at a considerably more detailed level than previously.

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I. INTRODUCTION

The theory of stellarator transport was originally developed as a number of somewhat disconnected expressions for transport coefficients, which were derived in different regimes of collision frequency ν and which cannot, as a result, be expected to match smoothly and correctly onto one another. In addition, a number of assumptions were made in order to obtain analytic results which substantially limit their validity. Most important among these are the ordering of characteristic time scales, and the conditions imposed to specify fully the distribution function f , particularly in the vicinity of the ripple-trapped boundary.

Up to now, numerical studies of stellarator transport have employed Monte-Carlo (M-C) codes. The early approaches [1,2] were guiding center M-C codes, whose promising results prompted a string of applications using this type of code (see, for example [3-7]).

Though effective in collisionality regimes down to the " $1/\nu$ " regime (for which diffusion coefficient $D \sim 1/\nu$), at lower collision frequency ν (in the "transitional" or "plateau" regime, where $D \sim \nu^0$ or $\nu^{1/2}$, and the "superbanana" regime, where $D \sim \nu$), computation time for the guiding center codes becomes unmanageably long. In order to be able to study these regimes numerically, which are of primary importance for ions in a fusion reactor, M-C codes have more recently been developed [8,9] in which the equations of motion are "bounce-averaged," i.e., averaged over the time for a particle to bounce in (or to transit) a ripple well. These codes have provided access to the lower ν regimes, and permitted numerical tests of analytic theories [10,11] applicable to those regimes.

However, the usefulness of even the bounce-averaged M-C codes in clarifying theoretical questions is limited, both because the run time at low

v is still long, and also because the connection between the orbit-following approach of the M-C codes and the p.d.e.-solving approach of kinetic theory is somewhat indirect. Accordingly, though a comparison can be made of $D(v)$ from both approaches, it is very difficult to check whether the two agree at the more detailed level of the form of the distribution function. Thus, even when theory and numerical experiment yield the same $D(v)$, one cannot know whether there is not an appreciable difference between the two at this more microscopic level, which could lead to significantly different predictions for $D(v)$ for different parameters. Moreover, when the predictions of theory and the bounce-averaged M-C results diverge, it is difficult to ascertain why.

The comparison between theory and these bounce-averaged M-C transport results indicated some areas of approximate agreement, and some anomalies. As an example of the latter, the transition from the $v^{1/2}$ to the $1/v$ regime was found to be flat, for v varying by over an order of magnitude [12], instead of the uninterrupted transition (reaching a larger maximum value) expected by existing theory. Another anomaly found in the M-C results was a significant enhancement of D at low v when the sign of the radial electric field E_r was switched from positive (the sign assumed in Ref. [11]) to negative. Other disparities, not only between theory and numerical experiment, but between the numerical results of different codes, appeared to exist in the character of the distribution function f in the vicinity of the boundary in pitch angle for ripple trapping, even when the corresponding transport results were in rough agreement. However, the statistics from the M-C codes were insufficiently precise to form a clear picture of f .

To provide an improved numerical tool for the study of stellarator transport, by which existing analytic transport theories may be evaluated and new theories developed, we have developed a bounce-averaged Fokker-Planck (F-

P) code FPSTEL, whose description and first applications are the subject of this paper. A major strength of the F-P approach is that its connection to analytic transport theory is considerably more direct than that for M-C codes. In both analytic theory and the F-P code, one solves the kinetic (Fokker-Planck) equation for f , and then computes the appropriate phase-space moment of f to obtain the desired fluxes and transport coefficients. Thus, a comparison between numerical and analytic results can be made with less uncertainty, and the appropriateness of the approximations used to make analytic progress are more directly suggested and tested.

A second advantage of the F-P approach is that it tends to be faster (experience indicates by a factor of 10 to 30) than the M-C codes. In part, this is due to the "Eulerian" character of the F-P code, i.e., the equations of motion are computed only once over the fixed grid at the beginning of a run. In contrast, M-C codes are "Lagrangian," i.e., at each time step on each particle orbit, the equations of motion must be recomputed. However, the constraints which physics places on required run times for both types of code are, of course, similar in many respects.

A final justification of the F-P approach is simply that it provides a complementary way of studying a complicated problem, giving an independent standpoint for evaluating results from other approaches.

While transport theory in the $1/\nu$ regime is relatively well-understood, in the less collisional $\nu^{1/2}$ and ν regimes, the analytic difficulties are considerably greater, and their proper solution more controversial. In this paper, we pay particular attention to the least collisional ($D \sim \nu$) regime, using the F-P code to test the validity of existing theory [10,11] in this regime in more detail than has previously been possible. The validity of theory in the transitional regime ($D \sim \nu^0$ or $\nu^{1/2}$) already mentioned will be

examined in a subsequent paper [13].

The remainder of this paper is organized as follows. In Sec. II we describe the theoretical considerations entering into the development of FPSTEL, including the development of the appropriate equations of motion and kinetic equation for the bounce-averaged problem, the manner in which we have dealt with the entrapping/detrapping process central to this kind of transport, and important properties of the kinetic equation, which one wants built into the code. In Sec. III we present numerical results from FPSTEL, and compare these with theoretical expectations and with results from the bounce-averaged M-C codes. Some summarizing comments are made in Sec. IV.

II. THEORY

We seek steady-state solutions of the Fokker-Planck (or Boltzmann) equation, which we write in conservation form:

$$\partial_t f + \nabla_z \cdot (\dot{z} f) = C f \quad (1)$$

Here, the six-dimensional phase space is parametrized by the variable set z^i ($i = 1, \dots, 6$), for the moment left unspecified. C is the (linearized) collision operator, and $\nabla_z \cdot$ denotes the divergence in phase space. For any vector $\underline{v}$ in phase space,

$$\nabla_z \cdot \underline{v} \equiv J^{-1} \partial_i (J v^i) \quad (2)$$

where $J \equiv |\partial(\underline{x}, \underline{p})/\partial \underline{z}|$ is the phase space Jacobian, $\partial_i \equiv \partial/\partial z^i$, $v^i \equiv \underline{v} \cdot \nabla_z z^i$ ($i=1, \dots, 6$) are the contravariant components of $\underline{v}$, and summation over repeated indices is implied. Due to the Hamiltonian character of the collisionless

equations of motion, $\dot{\mathbf{z}}(z)$ satisfies the Liouville property

$$0 = \nabla_{\mathbf{z}} \cdot \dot{\mathbf{z}} \equiv J^{-1} \partial_i (J z^i) \quad , \quad (3)$$

so that the $\dot{\mathbf{z}}$ in Eq. (1) may be commuted outside the divergence, if desired.

Now we begin to specify the z^i , reducing the number of relevant variables from six to two, paralleling what is done in analytic theory. We parametrize real space with flux coordinates (ψ, ζ, θ) , with $2\pi\psi$ the toroidal flux contained within a flux surface, and ζ and θ the toroidal and poloidal angles, respectively. Instead of ψ , it is sometimes more convenient to label flux surfaces with the minor radial variable $r(\psi) \equiv (2\psi/B_0)^{1/2}$, where B_0 is the field strength on axis.

In terms of the guiding-center variable set $z_1 \equiv (\psi, \zeta, \theta; \phi_g, \mu, E, \sigma)$, one has

$$dx dp = d\psi d\theta d\zeta (R/B) \sum_{\sigma} 2\pi M dE d\mu B/u \quad , \quad (4)$$

where $\sigma \equiv v_{\parallel}/|v_{\parallel}|$ is the sign of the parallel velocity, and $u \equiv |v_{\parallel}| = [2(E - e\phi - \mu B)/M]^{1/2}$ is its magnitude. E is the particle energy, e its charge, $\phi(r)$ the electrostatic potential, μ the magnetic moment, and M the particle mass. The factor of $2\pi = \oint d\phi_g$ in (4) is the only vestige of the gyrophase ϕ_g , so that ϕ_g henceforth drops from the problem. From (4), one reads off the Jacobian for the z_1 coordinate set:

$$J_1 = \sum_{\sigma} 2\pi M R/u \quad .$$

We introduce the usual model expression for the field strength B of a

stellarator,

$$B(\tilde{x}) = B_0 (1 - e_t - e_h \cos \eta) \quad , \quad (6)$$

with $e_t(r, \theta) = \epsilon_t(r) \cos \theta$ the toroidal perturbation, $e_h(r)$ the amplitude of the helical ripple perturbation, and $\eta \equiv n\zeta - m\theta$ the ripple phase.

In preparation for bounce averaging, we introduce well-depth parameter y ,

$$y(r, \theta; E, \mu) \equiv [(K/\mu B_0 - 1) + e_t + e_h]/2e_h \quad , \quad (7)$$

with $K \equiv E - e\phi$ the particle kinetic energy. From Eqs. (6) and (7) it follows that

$$u(\tilde{x}; E, \mu) = \hat{u}[y - \sin^2(\eta/2)]^{1/2} \quad , \quad (8)$$

where $\hat{u} \equiv 2(\epsilon_h \mu B_0 / M)^{1/2}$. From Eq. (8), one sees that $y = 0$ for a particle most deeply ripple-trapped ($u = 0$ at $\eta = 0$), $y = 1$ for a particle barely trapped ($u = 0$ at $\eta = \pm\pi$), and $y > 1$ for a toroidally trapped ("blocked") or passing particle. It is also useful to introduce the bounce action I ,

$$I(r, \theta, E, \mu) \equiv \int_0^{\pi} \int_h \frac{dl}{2\pi} \mu u = \hat{\mu} u L_h A(y) \quad , \quad (9)$$

where $\int_h dl$ denotes an integral along a field line across the h^{th} helical ripple well, and $2\pi L_h$ is the distance along the field across that well. The second form for I is obtained using u from Eq. (8). $A(y)$ is given by

$$A(y) \equiv \sum_{\sigma} \int_h \frac{dn}{2\pi} [y - \sin^2(\frac{n}{2})]^{1/2} \quad (10)$$

$$= \begin{cases} \frac{4}{\pi} [E(y^{1/2}) - (1-y)K(y^{1/2})] & , \quad y < 1 \\ \frac{4}{\pi} E(y^{-1/2})y^{1/2} & , \quad y > 1 \end{cases}$$

with K and E the complete elliptic integrals of the first and second kind, respectively. $A(y)$ has the limiting cases

$$A(y \ll 1) = y \quad , \quad A(1) = 4/\pi \quad ,$$

and

(11)

$$A(y \gg 1) = 2y^{1/2} \quad .$$

For $y < 1$, I is an adiabatic invariant of the collisionless motion, while for $y > 1$, I itself is not invariant. [Rather, the sum of the I -values over each ripple well a particle enters in the course of a toroidal bounce (or transit) is invariant.] For both $y < 1$ and $y > 1$, one has $u^{-1} = \partial_E(Mu)$, and therefore

$$\langle \sum_{\sigma} u^{-1} \rangle_h \equiv (\int_h \sum_{\sigma} d\ell/u) / \int_h d\ell = \partial_E I / L_h = (2/u) A'(y) \quad . \quad (12)$$

From Eq. (10), $A'(y) \equiv \partial_y A(y)$ may be evaluated:

$$A'(y) = \begin{cases} \frac{2}{\pi} K(y^{1/2}) & , \quad y < 1 \\ \frac{2}{\pi} K(y^{-1/2})/y^{1/2} & , \quad y > 1 \end{cases} \quad (13)$$

Averaging Eq. (4) over a ripple well yields a bounce-averaged Jacobian:

$$\langle dx \, dp \rangle_h = d\psi \, d\theta \, d\zeta \, d\mu \, dE \, \bar{J}_1 \quad , \quad (14)$$

where

$$\begin{aligned} \bar{J}_1 &= 2\pi \, MR \, \langle \int_{\sigma} u^{-1} \rangle_h \\ &= 2\pi RM^{3/2} (\epsilon_h \mu B_0)^{-1/2} A'(y) \quad . \end{aligned}$$

Again in parallel with analytic theory, we model the collision operator with the Lorentz operator, which scatters in pitch angle only:

$$\begin{aligned} C_L f &= v(u/B) \partial_{\mu} \mu u \partial_{\mu} f \\ &= (v_h u / 2\epsilon_h \mu B) \partial_y \mu u \partial_y f \quad , \end{aligned} \quad (15)$$

where $v_h \equiv v/(2\epsilon_h)$, and $\partial_y \mu \equiv -2\epsilon_h \mu$ has been used. In Eq. (15), ∂_{μ} and ∂_y are derivatives at constant ψ and E (or K). Thus, since the collisionless portion of the equations of motion also conserves E , E becomes simply a parameter in the problem, which must be integrated over to obtain a total radial flux from the flux coming from each constant energy shell at any specific radius.

Bounce averaging Eq. (15) across a ripple well, using Eq. (12) for the

helical bounce/transit frequency $\Omega_{bh} = (\partial_E I)^{-1}$,

$$\begin{aligned}\bar{c}_L f &\equiv \left(\sum_h \int_h \frac{d\ell}{u} c_{Lh} f \right) / \left(\sum_h \int_h \frac{d\ell}{u} \right) \\ &= (v/B) \left(\partial_\mu I u \partial_\mu f \right) / \partial_E I \\ &= v_h \left(\partial_Y A \partial_Y f \right) / A' \quad .\end{aligned}\tag{16}$$

The principal quantity of interest for transport theory is the radial flux density of particles and energy, which may be written

$$\Gamma_g^r \equiv (\Delta V)^{-1} \int_{\Delta V} d^6 z \, J \, g(E) \hat{r} \, f \quad .\tag{17}$$

Here, $g(E) = 1$ for the particle flux and $g(E) = E$ for the heat flux. Because we compute the flux for each energy shell, $g(E)$ is just a multiplicative parameter, so we shall set $g = 1$ henceforth. $\Delta V = (2\pi)^2 r R \Delta a$ is the volume of a toroidal shell, centered at the radius r of interest, and of thickness Δa , small compared with the minor radius a , and the scale lengths $L_a \sim a$ over which macroscopic quantities (such as temperature T or density n) vary appreciably. " ΔV " in $\int_{\Delta V}$ confines the phase space integral to that volume.

At this point we commit ourselves to γ in favor of μ as our pitch angle variable, as it aids physical clarity, and again follows the usual procedure in analytic theory. We thus use the variable set $z_2 = (r, \theta, \gamma; E, \zeta, \phi_g)$. The three variables following the semicolon have been eliminated from the problem. As in analytic theory, we eliminate a fourth, r , by the assumption that $\hat{r}$ is small, i.e., that $\hat{r} \partial_r \ll \partial_\theta \partial_\theta, \hat{y} \partial_\gamma$. We write $f = f_0 + f_1$, where

$f_0 = f_0(E, r)$ is the unperturbed distribution function, satisfying

$$Cf_0 = 0 \quad . \quad (18)$$

Using Eqs. (3) and (18), $f_0(E, r)$ in Eq. (1) contributes only a source term

$$S \equiv -\dot{r} \partial_r f_0 + \dot{r} f_0 / L_a \quad . \quad (19)$$

The final replacement in Eq. (19) may be taken as a definition of L_a , whose sign is positive.

Of the two terms in

$$J_2^{-1} \partial_r (J_2 \dot{r} f_1) = \dot{r} \partial_r f_1 + f_1 J_2^{-1} \partial_r (J_2 \dot{r}) \quad ,$$

the first is negligible in comparison with S . For $y > 1$, the second term is negligible in comparison with the terms in ∂_θ and ∂_y . From the equations of motion for $y < 1$ to be given shortly, one has

$$\partial_r (J_2 \dot{r}) = -2\partial_y (J_2 \dot{y}) = -2\partial_\theta (J_2 \dot{\theta}_B) \quad ,$$

where $\dot{\theta}_B$ is the grad-B contribution to $\dot{\theta}$, small compared with the $E \times B$ portion Ω_B . Using this property, the remaining term in $\partial_r (J_2 \dot{r})$ can be absorbed into the $\dot{\theta}$ term [cf. Eq. (27) and the discussion following]. Equation (1) may then be approximated by

$$\partial_t f + J_2^{-1} (\partial_\theta \gamma_O^\theta + \partial_y \gamma_O^y) - Cf = S \quad , \quad (20)$$

in which the ∂_r -term no longer explicitly appears (so that r is reduced to the status of a mere parameter), but in which the conservation properties of Eq. (1) are preserved. Here, $\gamma_0^i \equiv J_2^i f$, with the subscript "0" denoting its collisionless origin.

Using Eq. (14), one readily finds J_2 :

$$J_2 = \int_0^\pi 2\pi r R M^{3/2} K^{1/2} \epsilon_h^{1/2} A'(y) \quad , \quad (21)$$

where we have used $\mu B_0 = K$. As is $\bar{J}_1$ in Eq. (14), J_2 is a bounce-averaged quantity. The overbar is suppressed for notational simplicity. In cases where only the contribution from one sign of σ is desired, the $\int_\sigma$ in Eq. (21) should be dropped.

J_2 in Eq. (21) is independent of θ , and depends on y only through A' . Thus, one may cast Eq. (16) in the form

$$\bar{C}_L f = -J_2^{-1} \partial_y \gamma_v^y \quad , \quad (22)$$

where

$$\gamma_v^y \equiv -J_2 v_h (A/A') \partial_y f \quad .$$

Using Eq. (22), and defining $\gamma_v^\theta \equiv 0$, $\gamma^i \equiv \gamma_0^i + \gamma_v^i$, one can write Eq. (20) in conservation form:

$$\partial_t f + J_2^{-1} (\partial_\theta \gamma^\theta + \partial_y \gamma^y) = S \quad . \quad (23)$$

Because $S = \dot{r} \propto \sin \theta$ is odd in θ [cf. Eq. (25)], from Eq. (23) it is evident

that the total number of particles N is conserved:

$$0 = \dot{N} = \partial_t \int dz_2 J_2 f \quad (24)$$

Using the finite difference analogue of Eq. (23), this important property is built into FPSTEL. When the equations of motion do not conserve N well, the form of the resultant f can be substantially modified.

Collisionless Motion

The formulation thus far has treated ripple-trapped and untrapped particles on the same footing. The rather different physics between these two particle states enters in writing down explicit expressions for the $\dot{z}^i$, which we now do.

For both $y < 1$ and $y > 1$, we take

$$\dot{r} = v_B \sin \theta, \quad v_B \equiv K/M\Omega R \quad (25)$$

Here, $\Omega \equiv eB/Mc$ is the particle gyrofrequency, and we have again used the approximation $\mu B \approx K$, valid for $y \ll \epsilon_n^{-1}$, where the physics relevant to ripple transport occurs.

As has been noted, for $y < 1$, I is a constant of the motion. Taking $m = 2$ for simplicity, so that $\epsilon_n \sim r^2$, from Eq. (9) I -conservation implies $0 = d/dt[rA(y)] = \dot{r}A + rA'\dot{y}$, and thus

$$\dot{y}(y < 1) = -(\dot{r}/r)(A/A') \quad (26)$$

$\dot{\theta}(y < 1)$ has both an $E \times B$ and grad- B contribution:

$$\dot{\theta}(y < 1) = \dot{\Omega}_E - \dot{\theta}_B, \quad (27)$$

where $\dot{\Omega}_E \equiv eE_r/(M\Omega r)$ and $\dot{\theta}_B \equiv (v_B/r)\cos\theta$. One has $\dot{\theta}_B/\dot{\Omega}_E \sim \epsilon_t(e\phi/T) \ll 1$ for expected values of the radial potential $\phi(r)$ [14].

Though small relative to $\dot{\Omega}_E$, $\dot{\theta}_B$ is needed to preserve the important Liouville property (3). The physical $\dot{\theta}$, for which Eq. (3) is satisfied, is $\dot{\theta}_P = \dot{\Omega}_E + \dot{\theta}_B$. The reversal of the sign of $\dot{\theta}_B$ in going from $\dot{\theta}_P$ to $\dot{\theta}$ in Eq. (27) is due to the absorption into the term $\partial_\theta(J_2\dot{\theta})$ of the contribution from $\partial_r(J_2\dot{r})$ in Eq. (3). Using Eqs. (21), (26), and (27) it is easily verified that our approximate equations of motion for $y < 1$ exactly satisfy

$$0 = \partial_\theta(J_2\dot{\theta}) + \partial_y(J_2\dot{y}) \quad (28)$$

the same as the exact relation (3) specialized to $z = z_2$, but with the $\dot{r}$ -term missing. Thus, with S "shut off," a steady-state solution of Eq. (20), annihilated by both the collision operator and the Liouville operator [the terms in γ_0^1 in Eq. (20)], is an f constant over the (θ, y) plane, i.e. $f = f_0(E, r)$. As for particle conservation, it is important that the finite-difference analogue of Eq. (28) be built into the F-P code. If not well-obeyed, nonphysical contributions to f result which can produce spurious transport, particularly at extreme values of collisionality, where the physical transport is small.

For $y > 1$, $\dot{\theta}$ is dominated by its free-streaming portion

$$\dot{\theta}(y > 1) = \sigma_1 \bar{u}/R \quad (29)$$

Here, $\bar{u}(y)$ is the parallel velocity u , time averaged over a ripple well transit, and $\mathbf{i}$ is the rotational transform. Using Eq. (12),

$$\bar{u} = 2 \langle \epsilon u^{-1} \rangle^{-1} = \hat{u}/A' \quad (30)$$

Finally, with the usual approximation that r is about constant for a particle with $y > 1$, Eq. (7) determines $\dot{y}$ in terms of $\dot{\theta}$. Thus,

$$\dot{y}(y > 1) = \partial(\partial_{\theta} y) = -\dot{\theta} \sin \theta/2p \quad (31)$$

where $p \equiv \epsilon_h/\epsilon_t$. From Eqs. (21), (29), and (31), it follows that

$$\partial_{\theta}(J_2 \dot{\theta}) = 0 = \partial_y(J_2 \dot{y}) \quad (32)$$

so that Eq. (28) holds for $y > 1$ as well.

The character of the collisionless orbits in the (θ, y) plane is shown in Fig. 1a for $E_r > 0$, and Fig. 1b for $E_r < 0$. As discussed in Ref. 11, the trajectory $y_{dt}(\theta)$ divides superbanana orbits which never detrapp ($y < y_{dt}$) from those which do, while the trajectory $y_{tp}(\theta)$ divides toroidally trapped from passing particles. These limiting orbits are approximately described by [11]

$$y_{dt}(\theta) = 1 + (\cos \theta - 1)(\Delta r_1/r) \quad (33)$$

and

$$y_{tp}(\theta) = 1 + (\cos \theta + 1)/(2p) \quad (34)$$

Here, $\Delta r_1 \equiv v_B/\Omega_E$ is the amplitude of the radial excursion of a superbanana. The arrowheads on the trajectories indicate the direction of particle motion. Above $y = 1$, the arrows point in both directions, corresponding to the two signs of σ in Eq. (29). Thus, FPSTEL must keep track of three domains of f . We write $f = f_\tau$, where the index τ takes on three values: $\tau = r$ for ripple-trapped particles, $\tau = f$ for forward moving particles ($\sigma = 1, y > 1$), and $\tau = b$ for backward moving particles ($\sigma = -1, y > 1$). From the direction of $\theta(y < 1)$ in Figs. 1, one notes that entrapping occurs for $\theta > 0$, and detrapping for $\theta < 0$. The numerical results for $f(\theta, y)$ presented here will follow this convention.

Collisionless Entrapping/Detrapping

We have seen that the approximate equations of motion for both $y < 1$ and $y > 1$ satisfy the Liouville condition (28) for incompressible flow, so that in the absence of the driving term S , an f constant over the (θ, y) plane is a steady-state solution. However, one must also ensure that the flow be incompressible across $y = 1$, or again one finds a nonphysical distortion of f , corresponding to a pileup or depletion of f in the neighborhood of $y = 1$. Since all particles in the interval $y_{dt} < y < 1$ will detrap, the detrapping flux for $\theta < 0$ is known, and this must be precisely balanced, in steady state, by the entrapping flux at $\theta > 0$. The entrapping probability P_{er} ($\tau = f + r$) for collisionless particles may be calculated in essentially the same manner as done by Goldston and Towner [15] for entrapping in rippled tokamaks. For the present considerations, where $\alpha \equiv e_t/n_{eh} \ll 1$, and the $E \times B$ drift dominates the grad-B drift in the entrapping process, the result is

$$P_{er} = (\Omega_E L_h / 2\pi u) \cot(\theta) P(0) / \sqrt{2} \quad , \quad (35)$$

where $P(0) = 2\pi^3$ is defined as in Ref. [15].

Although a useful theoretical result, because even a small mismatch between the detrapping and entrapping rates can lead to appreciable distortion of f , in FPSTEL P_{fr} is instead determined by matching the y -fluxes when $f_F = f_r$ on neighboring meshpoints on either side of the $y = 1$ boundary:

$$P_{fr} = J_2 \dot{y}(\theta, 1 - \Delta y/2) / J_2 \dot{y}(\theta, 1 + \Delta y/2) \quad , \quad (36)$$

with Δy the mesh spacing in y . This rigid requirement that P_{fr} satisfy the Liouville condition is a noteworthy difference between the present F-P code and bounce-averaged M-C codes, where P_{fr} may be set to any value between 0 and 1, without anything obviously pathological happening. On the one hand, this greater flexibility of the M-C codes permits an examination of the effect of P_{fr} on transport, which analytic work [11,16] indicates can be significant. On the other hand, since P_{fr} is in fact determined by the Liouville property, it is useful to have violations of this physical requirement made manifest.

The connection between Liouville's theorem and the trapping probability is clarified in Fig. 2, where we show the incompressible flow projected into the (θ, ζ) plane, for particles having the same K and μ , but distributed in θ and ζ . For a given K/μ , particles reflect from points $\tilde{x}$ in the flux surface where $B(\tilde{x}) = B_1 \equiv K/\mu$. In a contour plot using model (6), B_1 contours would be parabolically shaped curves, centered on the lines $\eta = (2i + 1)\pi$ of maximum ripple strength, and with vertices on that line at the value of θ where $y = 1$. For clarity, we idealize these B_1 contours, representing them by the $\eta = (2i + 1)\pi$ axes on which the real contours would be centered, which one may regard as barriers from which incoming particles reflect.

We have chosen $\Omega_E > 0$ here, and show only the entrapping side ($\theta > 0$). Detrapping is simply the time-reversed process. We focus on the band of incoming ($\sigma = 1$) trajectories, delimited by the trajectories a and b, which will entrap on the present bounce. At constant θ , this band subtends toroidal angle $\Delta\zeta_r$, while the rest of those trajectories reflecting in the single field period shown subtend an angle $\Delta\zeta_b$. From the figure one sees that $P_{fr} = \Delta\zeta_r / (\Delta\zeta_r + \Delta\zeta_t)$. The size of $\Delta\zeta_r$ is proportional to the small angle which the trajectories make with the magnetic field, which is in turn proportional to the drift Ω_E . By our choice of orbits a and b, it is also clear that after its second bounce, orbit a lies precisely adjacent to orbit b, so the $r = r$ region is completely filled by the incoming flux from the a-b band. The Liouville condition ensures that f is constant all along this band, as it is along the complementary band of particles which do not entrap ($r = f + b$).

Some Other Considerations

In the interior of the domains $r = f, b, r$, particle conservation is ensured by the finite-difference counterpart of the divergence theorem. For example, for the θ -flux

$$\theta = \sum_{l_0} [\gamma^\theta(\theta + \Delta\theta, y) - \gamma^\theta(\theta - \Delta\theta, y)] / (2\Delta\theta) \quad , \quad (37)$$

where $\theta = i_0 \Delta\theta$. Thus, the θ flux at each mesh point is added and subtracted once. The same property holds for the y -flux, except at $y = 0, 1$, and y_u , where y_u is the upper limit of y kept in the grid. At these y -values, care must be taken that γ^Y from each meshpoint on these boundaries is added and subtracted once. From Eqs. (26) and (11) one sees that $\dot{y}(y=0) \neq 0$, so the boundary at $y = 0$ contributes no y -flux. At $y = 1$, the incoming flux

$\gamma_f^y(\theta, 1+\Delta y/2)$ from f_f contributes an amount $P_{fr}\gamma_f^y$ to the entrapping distribution $f_r(\theta, 1-\Delta y/2)$, and an amount $P_{fb}\gamma_f^y$ to the reflected distribution $f_b(\theta, 1 + \Delta y/2)$, where

$$P_{fr} + P_{fb} = 1 \quad . \quad (38)$$

If Eq. (38) is satisfied, $\gamma_f^y(\theta, 1+\Delta y/2)$ is again added and subtracted once in the sum over all mesh points. The confluence at $y = 1$, $\theta < 0$ of f_r and f_b is handled similarly.

At $y = y_u$, N-conservation is maintained by identifying as a nearest neighbor of the point at (θ, y) the point at $(-\theta, y)$, instead of the point at $(\theta, y+\Delta y)$ which would be used in the interior, but which is out of bounds for the mesh. Thus, particles flowing out the top of the mesh at (θ, y_u) immediately reappear at $(-\theta, y_u)$. For y_u sufficiently large, f should be little modified, so little physics should be lost.

The split of f_f into f_b and f_r for $\theta > 0$, and the recombination of f_b and f_r into f_f for $\theta < 0$ point to one respect in which our approximate equations of motion are oversimplifications. As has been discussed, for S in Eq. (20) set to zero, a steady-state solution for both $y > 0$ and $y < 0$ is $f = f_0(E, r)$, a constant over the (θ, y) plane. However, f_0 cannot be the same constant for $\tau = b$ as for $\tau = f, t$. If it were, Eq. (29) would imply that the "back flux" in θ would exactly cancel the forward flux,

$$\Gamma_b^\theta = -\Gamma_f^\theta \quad , \quad \Gamma_\tau^\theta \equiv \int dy \gamma_\tau^\theta \quad .$$

This would violate particle conservation, since a fraction P_{fr} of the forward flux must be going into Γ_r^θ . Thus, the expressions for $\dot{z}^i$ given above have a

collisionless, steady-state, "unperturbed" ($S = 0$) distribution f_0 given by

$$f_{0r} = f_{0f} \equiv f_0, \quad f_{0b} = P_{fb} f_0 \quad . \quad (40)$$

To assure that Eq. (40) is a solution for $v > 0$ as well, the finite-difference form of C across $y = 1$ must correspondingly be slightly modified from its more standard form elsewhere on the grid, by the replacement of f_b by the slightly larger f_b/P_{fb} , wherever it occurs in C .

This small deviation from the physically expected steady-state $f_r = f_0$ ($r = f, b, r$) occurs because the small drift term Ω_E [which, as one sees from Eqs. (35) and (36) and Fig. 2, is crucial in providing the ripple-trapped flux] is absent in Eq. (29). Simply adding Ω_E to Eq. (29) is physically plausible, but leads to the violation of the Liouville property Eq. (28). More satisfactory modifications of this sort are presently under study.

III. NUMERICAL RESULTS

In the results presented here, we restrict ourselves to consideration of a single set of machine parameters. We take $B_0 = 5$ Tesla, $R = 10$ m, $a = 2$ m, so that $\epsilon_t(r/a = 0.5) = 0.1$. Also, $\epsilon_h(r/a = 0.5) = 0.075$, and $n = 5$, so that $i = 1.8$. The radial flux is computed at $r/a = 0.5$. We take a rather energetic plasma, $K \approx T_i = 50$ keV, and $eE_{ra}/T_i = \pm 2$. The large value of T_i provides an appreciable superbanana width while not allowing $\dot{\theta}$ for $y > 1$ and $y < 1$ to become too disparate, as this increases the computation time required. Typically $\dot{\theta}(y > 1) \sim 2 \times 10^5 \text{ sec}^{-1}$, and thus $\dot{\theta}(y > 1)/\dot{\theta}(y < 1) \sim$

20.

Using a time-centered implicit scheme, f is advanced in time until it and the radial flux Γ^r it produces have settled down. For a given f , Γ^r is

directly computed from the discretized version of Eq. (17), and the conversion factor from Γ^r to diffusion coefficient $D(K)$ for a given energy shell is obtained by comparing Eq. (17) with the defining equation for D [11]:

$$\Gamma_g^r = - \sqrt{2} \, 4\pi \, M^{-3/2} \int dk K^{1/2} g D(K) \partial_r f_o \quad . \quad (41)$$

In Fig. 3 we plot D versus collisionality, parameterized by density n and v_h/Ω_E . Solid dots denote numerical points for $E_r > 0$, and open circles designate $E_r < 0$. Half-open, half-solid circles indicate essentially identical values for both signs of E_r . For the present parameters, at least, one notes that transport is insensitive to the sign of E_r . The light curves show the predictions of theory in the linear superbanana regime (D_1), transitional $v^{1/2}$ regime ($D_{1/2}$), $1/v$ -regime (D_{-1}), and tokamak banana regime (D_{bn}). As D_{bn} arises from a separate transport mechanism, the total transport (denoted by the heavy curve D) is the sum of D_{bn} and the appropriate one of D_1 , $D_{1/2}$, and D_{-1} .

At low collisionality ($v_h/\Omega_E \lesssim 0.05$) one observes a roughly linear regime, with magnitude in approximate agreement with theory [11], whose locus is marked with the theoretical curve D_1 . The points for $E_r > 0$ follow the D_1 curve slightly better than those for $E_r < 0$, which appear to have a small additional contribution scaling more weakly than v . This may be due to an additional boundary layer contribution, discussed in [8] and [16]. For v_h/Ω_E above 0.05, the numerical results follow well the theoretical curve $D(v)$ through the $v^{1/2}$ regime, and into the $1/v$ regime, where the $1/v$ ripple behavior is partly masked by the comparable size of D_{bn} . Above $v_h/\Omega_E = 4$, however, the numerical points fall well below the curve $D = D_{-1} + D_{bn}$ for total transport, while remaining well above the ripple contribution D_{-1} .

alone. Since our equations of motion have been averaged only over a helical ripple well, one expects the code to be able to register the banana regime. We believe the deviation of the numerical points from D in the banana regime $D \approx D_{bn}$ is largely due to the maximum y value $y_u = 3$ taken on the grid. While large enough to capture most of the interesting ripple transport (the main intent here), since $y_{tp}(\theta = 0) = 2.33$ for these parameters, much of the region for particles nearly toroidally trapped is thus truncated, or significantly affected, by the boundary at $y = y_u$. This belief is supported by the fact that the perturbed distribution function f_1 found numerically is still quite appreciable at $y = 3$ at this collisionality. Additionally, when y_u was raised from 3 to 5 at $n = 5 \times 10^{23}$, for example, transport increased by about 38%. At lower ν , the measured transport is fairly insensitive to the value chosen for y_u . At $n = 10^{21}$, for example, D drops only about 10% in changing from $y_u = 3$ to $y_u = 2$. Since $y_{tp}(\theta=0) = 2.33$ for these parameters, $y_u = 2$ is a rather drastically small value. However, it is also possible that the difference between the theoretical curve and the numerical results in the banana regime is due in part to a physical effect, in which the presence of two different transport mechanisms, both of which give rise to a component of f varying as $\sin\theta$, interact with each other in such a way as to reduce transport below the level for the axisymmetric mechanism alone. This is especially true since no theory in which this interaction has been seriously dealt with exists at present.

Around the peak at $\nu_h/\Omega_E \approx 0.8$ in the transitional regime, agreement between theory and the results from FPSTEL in Fig. 3 is improved if one modifies [12] the $\nu^{1/2}$ -regime theory of Galeev and Sagdeev [10], by extending their analytic results to the case in which the collisional boundary layer $\Delta y_\nu \approx (\nu_h/\Omega_E)^{1/2}$ central to the $\nu^{1/2}$ theory becomes larger than the total width in

phase space $\Delta y = 1$ of the ripple-trapped particles. A more detailed study of this regime, comparing F-P results with theory for both D and f , will be presented in Ref. 13.

The Distribution Function

The transport results $D(v_h/\Omega_E)$ in Fig. 3 are of the standard sort presented in previous numerical approaches [1-9] to stellarator transport. However, D represents only a single moment of the distribution function, and so is only a crude measure of whether a given analytic theory has properly solved the kinetic equation for f . As noted in the Introduction, one of the strengths of the F-P approach is that it produces f directly, so that a more detailed check on theory is possible.

In Figs. 4 we show a first example of this, a contour plot of f over the (θ, y) plane for $v_h/\Omega_E = 2.2$, in the $1/v$ regime. Fig. 4a shows f_f and f_r , while Fig. 4b shows f_b and f_r . One notes the slight jump at $y = 1$ between the steady-state f_b and f_r in Fig. 4b, whose origin was discussed in Sec. II. Here, as in all cases we have examined thus far, the $\tau = r, b$ plots are otherwise similar to the $\tau = r, f$ plots. The grid used for this run is $n_\theta = 11$ points across by $n_y = 30$ points high, which gives adequate resolution at this v .

At any given y -value below $y = 1$ in Figs. 4, f_1 is sinusoidal, with $f_1 < 0$ for $\theta < 0$ (dotted curves), and $f_1 > 0$ for $\theta > 0$ (solid curves).

In the present notation, the theoretical result [17] for the perturbed distribution function $f_1 \equiv f - f_0$ in this region is

$$f_1 = \begin{cases} (\dot{r}/v_h)(y-1)\partial_r f_0 & , \quad y < 1 \\ 0 & , \quad y > 1 \end{cases} \quad (42)$$

This is plotted in Fig. 5 for the same parameters as in Fig. 4. One sees that Eq. (42) and the numerical solution agree well below $y = 1$. The main difference is that while f in Fig. 5 is precisely odd about $\theta = 0$, in Fig. 4 this sinusoidal shape is shifted slightly to the right. This shift is due to Ω_E , which is neglected in analytic theory. Above $y = 1$, the F-P result varies by an amount small compared with the variation below $y = 1$, so the usual analytic assumption that $f_1 = 0$ above $y = 1$ is reasonably well justified.

At low collisionality, the assumption $f_1(y > 1) = 0$ is invalid, and in general leads to incorrect solutions for f and for D . The mathematics of transport in this regime is made more difficult than analogous calculations in simpler situations (e.g., tokamak banana transport) by the more complicated, two-state character of the detrapping superbanana orbits ($y_{dt} < y < y_{tp}$). These are the dominant contributors to transport, within the idealizations [c_h in Eq. (6) θ -independent, and $\Omega_E \gg \dot{\theta}_B$] usually made in this regime. In particular, the probabilistic character of the retrapping process introduced by the bounce averaging makes it less apparent how one properly solves the kinetic equation for f_1 . In Refs. [11,16] an analytic prescription for solving for f_1 is developed, in which this probabilistic character is dealt with. As usual in low- ν theories, a subsidiary ordering in ν is introduced, $f_1 = f_1^0 + f_1^1$, where

$$f_1^0 = -\delta r(\theta, y) \partial_r f_0, \quad (43)$$

and

$$f_1^1 = \int^\theta d\theta' \langle \dot{\theta} \rangle^{-1} C f_1^0. \quad (44)$$

$f_1^0 \sim O(v^0)$ is the collisionless portion of f_1 , yielding no transport. Net transport comes from the smaller $f_1^1 \sim O(v)$. The theoretical difficulty lies in fully specifying the radial excursion $\delta r \equiv \int^\theta d\theta' (\dot{r}/\dot{\theta})$. Here and in Eq. (44), the integral $\int^\theta d\theta' (\dot{\theta})^{-1}$ is a time integration along the "unperturbed" trajectories of Fig. 1, i.e., along trajectories with $v = 0 = \dot{r}$, and $(\dot{\theta}, \dot{y})$ as given in Sec. II. Labeling these trajectories with a function $w(y, \theta)$ which is constant along them, one notes that the definition of δr just given is determined only up to an arbitrary function of w , $\delta r \equiv r(\theta, w) - r_G(w)$, with $r(\theta, w)$ the radial position of a particle on trajectory w at azimuth θ , and $r_G(w)$ the as yet undetermined function. In analytic theory, r_G is to be determined by the integrability condition

$$0 = \oint d\theta (\dot{\theta})^{-1} \bar{C} \delta r \quad (45)$$

Summarizing briefly, in Refs. [11,16] the integration over a closed orbit in Eq. (45) is divided into two portions, an integral over the time τ_r a particle on that orbit spends ripple-trapped, and an integral over the time $\tau_t \approx \tau_{bt}/P_{fr}$ it spends untrapped. (τ_{bt} is the toroidal bounce time.) Analytic solutions are tractable in the two limits $\tau_t \ll \tau_r$ and $\tau_t \gg \tau_r$. In the former case, the limit commonly assumed, Eq. (45) is satisfied by $r_G(w) \approx r_x(w)$, the maximum radius $r(\theta, w)$ attained for a given w , and in the latter case, the solution is $r_G(w) \approx r_n(w)$ the minimum radius attained (namely, the radius of the untrapped portion of the orbit).

These limiting solutions for $f_1^0 = \delta r$ are shown in Fig. 6 ($\tau_t \ll \tau_r$) and Fig. 7 ($\tau_t \gg \tau_r$). Above $y = 1$, the contours in Fig. 6 follow the collisionless trajectories of Fig. 1, due to the (approximate) independence of $r(\theta, w)$ from θ for $y > 1$. If $r_G(w)$ were modified continuously from the $r_x(w)$

of Fig. 6 to the $r_0(w)$ of Fig. 7, the contours above $y = 1$ would maintain their shape, but decrease in number, as $\delta r(y > 1)$ approached the constant value it has in Fig. 7.

In fact, for the present parameters one has $\tau_e/\tau_r \approx 0.8$, an intermediate case. Thus, one expects f_1^0 to have the character of the intermediate case just described. In Figs. 8 is shown f generated by FPSTEL, for $E_r > 0$ and $v_h/\Omega_E = 0.055$. Fig. 8a shows f_f and f_r , and Fig. 8b shows f_b and f_r . For low- v runs such as this one, it is important to have some resolution across the interval $y_{dt} < y < 1$ of ripple-detrapping superbananas. From Eq. (33), the width of this interval is $2\Delta r_1/r = 0.2$. Thus, $n_y = 120$ for $y_u = 3$ gives a grid spacing $\Delta y = 0.05$, adequate to resolve this region.

One notes that the even (about $\theta = 0$) portion of f in Fig. 8 has the character described above for the case $\tau_e/\tau_r \sim 1$. The contours above $y = 1$ roughly follow the unperturbed trajectories, but are somewhat less dense than in Fig. 6. Superposed on this is a small odd portion, which is identified with f_1^1 .

In the process of converging to a steady value of D , f takes on the appearance of $f_0 + f_1^0$ in Fig. 6 on a collisionless time scale $\sim \Omega_E^{-1}$. Thereafter, however, the odd portion of f , and accordingly D , continue to oscillate, reaching stable values on the longer collisional time scale $\sim v_h^{-1}$. The analytic ordering of the kinetic equation is thus reflected in the time evolution of the numerical solution.

The appearance of f for the $E_r < 0$ case is quite similar to that of Fig. 8, except that the form $f(y < 1) \propto -\cos\theta$ (minimum near $\theta = 0$, maximum near $\theta = \pm\pi$) is inverted in sign, as expected physically. This is shown in Figs. 9a and 9b, which are for the same parameters as in Figs. 8a and 8b, except for the reversal in sign of E_r . For neither case is any singular behavior noted

in f in the vicinity of $y = 1$, in contrast to indications of peaks [8] or depressions [9] reported from the M-C codes. When P_{fr} is not set as in Eq. (36) to allow the flow to satisfy the Liouville condition, peaks and depressions around $y = 1$ are indeed seen in the F-P results as well. Whether FPSTEL [using Eq. (36)] will show this singular behavior for physical reasons also, e.g., by changing device parameters or increasing the y -resolution, is still under investigation.

Earlier results using a bounce-averaged M-C code gave values for $D(v)$ which were roughly twice as large as expected theoretically (or found from FPSTEL) for $E_r > 0$, for the three low- v ripple transport regimes discussed here. For $E_r < 0$, the M-C code found still larger transport in the least collisional of these [8]. However, an upgrade of the M-C code to treat the entrapping/detrapping process more carefully by following (non-bounce-averaged) guiding-center orbits in the vicinity of $y = 1$ [18] has yielded preliminary results in which these disparities disappear. It may be, therefore, that the essential connection between the Liouville condition and P_{fr} is manifesting itself in the M-C results as well.

IV. CONCLUSION

We briefly summarize the discussion of the preceding sections. We have developed a computer code for solving the bounce-averaged F-P equation appropriate to stellarator transport for the distribution function f on a specified flux surface r , and for a single energy shell. This is in close correspondence with what is done in analytic theory, but is much less constrained by the need to make assumptions about parameter orderings or to impose questionable boundary conditions on f than is analytic theory. It has proven important that the code maintain properties of the exact kinetic

equation, such as particle conservation and the Liouville property of incompressible flow, and these have been built into the code. The importance of satisfying the Liouville property at the ripple-trapped boundary $y = 1$ has forced a clearer recognition of the direct relation between Liouville's theorem and the trapping probability than has been given in previous work.

Numerical results of two sorts have been presented, the plot of transport rates versus collisionality (Fig. 3) common to previous M-C and analytic studies, and plots of f over the (θ, y) plane, which permit a more detailed comparison between analytic theory and numerical experiment than previously possible. The transport results are in approximate agreement with theory over a broad range of collisionality. The theoretical expectations for f in the $v^{1/2}$ and $1/v$ regime are approximately borne out by the numerical results. In the linear superbanana regime, an analytic description for f really exists only in the limits $\tau_t \ll \tau_r$ and $\tau_t \gg \tau_r$ [11], while typically, and for the parameters used here, one has $\tau_t \sim \tau_r$. The numerical result for f in this intermediate case does look like what one would expect by interpolation between the two analytic limits, however, and so supports the theory in this approximate fashion. The F-P results for f in this regime are also in agreement with theory, and in contrast to the earlier M-C results, in not showing any particular peaking across the $y = 1$ boundary.

Finally, the theory in Ref. 11 was developed with $E_r > 0$ in mind. Owing to the topological difference in collisionless orbits between the two signs of E_r illustrated in Figs. 1, it is unclear that the expression for D developed in [11] applies to $E_r < 0$ without modification. However, the numerical results presented here suggest that this is approximately the case, though some evidence of a small additional boundary-layer contribution for $E_r < 0$ is discernable. This is currently being studied further.

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FIGURE CAPTIONS

FIG. 1. Depiction of the collisionless trajectories over the (θ, y) phase plane for radial electric field $E_r > 0$ (Fig. 1a) and $E_r < 0$ (Fig. 1b). $y = 1$ marks the entrap/detrapping boundary, $y = y_{dt}(\theta)$ marks the boundary between superbananas which do not detrapping ($y < y_{dt}$) and those which do, and $y = y_{tp}(\theta)$ marks the boundary between toroidally trapped ($1 < y < y_{tp}$) and passing ($y > y_{tp}$) particles.

FIG. 2. Illustration of the collisionless entrapping process, showing the projection into a flux surface of a family of trajectories with the same K and μ , but distributed in θ and ζ . See Sec II. for details.

FIG. 3. Plot of diffusion coefficient D versus collisionality, expressed in terms of density n (bottom scale) and v_h/Ω_E (top scale). Light lines indicate the predictions of theories valid in the various collisionality regimes covered by the plot, and the heavy line indicates the total transport expected theoretically. Solid dots denote numerical points for $E_r > 0$, open circles denote those for $E_r < 0$, and half-open, half-filled circles denote points where the $E_r > 0$ and $E_r < 0$ numerical results are essentially identical.

FIG. 4. Contour plot of the distribution function f generated by FPSTEL in the $1/\nu$ regime, $v_h/\Omega_E = 2.2$. Solid contours are used for $f_1 > 0$ and dotted contours for $f_1 < 0$. Figure 4a shows the forward-going distribution f_f for $y > 1$, and Fig. 4b shows the back-going distribution f_b .

FIG. 5. Contour plot using the same parameters as Fig. 4, for the distribution expected from analytic theory for the $1/v$ regime.

FIG. 6. Contour plot of the even part of the distribution expected from analytic theory in the linear superbanana regime, in the limit $\tau_t \ll \tau_r$.

FIG. 7. Contour plot of the even part of the distribution expected from analytic theory in the linear superbanana regime, in the limit $\tau_t \gg \tau_r$.

FIG. 8. Contour plot of the numerically generated distribution f in the linear superbanana regime ($v_h/\Omega_E = 0.055$), for $E_r > 0$. Figure 8a displays f_r and f_f , and Fig. 8b shows f_r and f_b .

FIG. 9. Same as Fig. 8, but for $E_r < 0$.

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Fig. 1

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Fig. 2

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Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7

#85T0169

Fig. 8

Fig. 9

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