

## ANNEX 32

### Test-particle simulations of ion drift in stochastic magnetic fields

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#### INTRODUCTION

Turbulence induced stochastic magnetic fields perturb the regularly nested magnetic field structures in toroidal confinement devices. They thus open new channels through which particles can potentially be transported and possibly give rise to enhanced or even anomalous particle diffusion. The resulting particle transport can be expected to depend on the level of the stochastic perturbations and on their spatial correlations. Here, we investigate the influence of the stochastic perturbations on transport by performing test-particle simulations in numerically generated stochastic magnetic fields, from which we determine the running diffusion coefficients. The stochastic fields are generated (i) with prescribed Gaussian distribution of varying standard deviation, and (ii) with prescribed spatial auto-correlation of Gaussian shape and fixed correlation length, and they are superimposed on a strong and uniform background magnetic field.

The results of the test-particle simulations are also compared to and used to validate the results as obtained for the same physical system by the semi-analytical Decorrelation Trajectory (DCT) method.

#### THE SET-UP

We consider a slab geometry, where the magnetic field  $\mathbf{B}$  is assumed to have a strong background component  $B_0$  in the  $Z$ -direction (in Cartesian coordinates  $X$ ,  $Y$  and  $Z$ ), and stochastic components in the perpendicular direction,  $\mathbf{B}(\mathbf{X}; Z) = B_0\{\mathbf{e}_Z + \beta b_X(\mathbf{X}; Z)\mathbf{e}_X + \beta b_Y(\mathbf{X}; Z)\mathbf{e}_Y\}$ , with the dimensionless  $\beta$  determining the strength of the perturbations,  $b_X$  and  $b_Y$  the normalised stochastic fields, and  $\mathbf{X}=(X, Y)$ .

In the parallel direction, we assume the particles to move as

$$\frac{dZ}{dt} = V_{\parallel} \quad (1)$$

where  $V_{\parallel}$  is the parallel velocity, and, for simplicity, we assume  $V_{\parallel}$  to be constant and to equal the thermal velocity  $V_{th}$ . The  $Z$  coordinate thus plays a dummy role, and we use it in the following instead of time  $t$ . We furthermore normalise the spatial coordinates with the correlation lengths  $\lambda_i$ ,  $i=X, Y, Z$  (defined below),  $x := X/\lambda_X$ ,  $y := Y/\lambda_Y$ ,  $z := Z/\lambda_Z$ .

For a stationary magnetic field, the linearised guiding centre equations of motion in the perpendicular direction can be written as (see [1], [2])

$$\begin{aligned} \frac{dx(z)}{dz} &= K_m b_x(\mathbf{x}; z) - K_{dr} \frac{\partial b_y(\mathbf{x}; z)}{\partial z} \\ \frac{dy(z)}{dz} &= \Lambda K_m b_y(\mathbf{x}; z) + \Lambda K_{dr} \frac{\partial b_x(\mathbf{x}; z)}{\partial z} \end{aligned} \quad (2)$$

where  $K_m = \beta\lambda_X/\lambda_Z$  is the magnetic Kubo number,  $\Lambda = \lambda_X/\lambda_Y$  the stochastic anisotropy parameter,  $K_{dr} = \beta V_{th}/\Omega\lambda_X$  the drift or thermal Kubo number, and  $\Omega = eB/mc$  the gyro-frequency. The system of equations is numerically integrated with a fourth order Runge Kutta, adaptive step-size scheme.

The running diffusion coefficients for the motion of the ions in the magnetic field are determined as

$$D_{xx} = \frac{\langle (x(z) - x(0))^2 \rangle}{2z}, \quad D_{yy} = \frac{\langle (y(z) - y(0))^2 \rangle}{2z} \quad (3)$$

where the averaging is taken over a large number of test particles.

## THE STOCHASTIC MAGNETIC FIELD

The spatial auto-correlation function  $M$  of the stochastic part  $\mathbf{A}_S=(0,0,A_z)$  of the vector potential is assumed to factorise,  $M(X,Y,Z) = M_X(X)M_Y(Y)M_Z(Z)$ , and to be of Gaussian shape for each of the coordinates,

$$M_X(X) \propto \exp[-X^2 / 2\lambda_X^2], \quad M_Y(Y) \propto \exp[-Y^2 / 2\lambda_Y^2], \quad M_Z(Z) \propto \exp[-Z^2 / 2\lambda_Z^2]$$

where  $\lambda_i, i=X,Y,Z$ , are the correlation lengths in the  $X, Y$ , and  $Z$  direction, respectively.

To construct the vector potential  $A_Z$  itself, we make use of the Wiener-Khinchine theorem. We first Fourier-transform  $M(X,Y,Z)$ , which yields  $M^*(k_x, k_y, k_z)$ , and the Fourier transform  $A_Z^*$  of  $A_Z$  is then given as

$$A_Z^* = \left| M^*(k_x, k_y, k_z) \right|^{1/2} \exp[i\varphi_{k_x, k_y, k_z}] \quad (4)$$

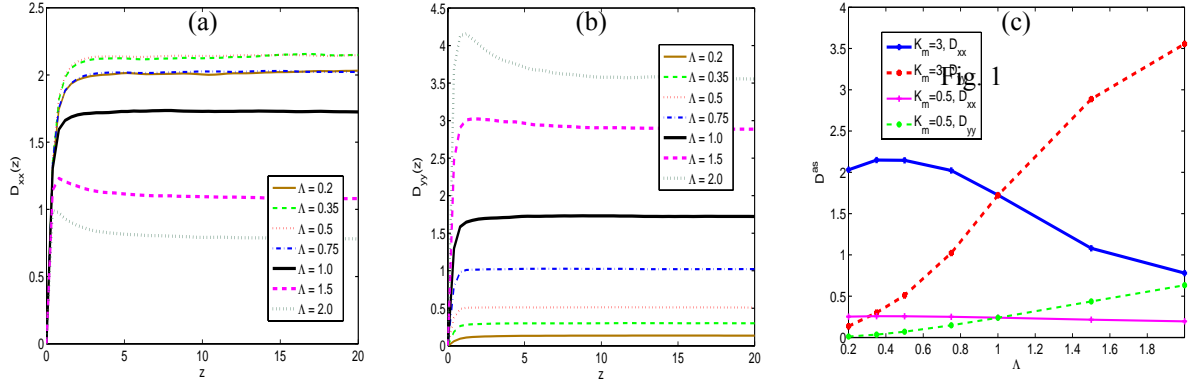
with the phases  $\varphi_{k_x, k_y, k_z}$  chosen uniformly random in  $[0, 2\pi]$ , and from which  $A_Z$  is determined by Fourier inverse-transformation. Derivatives of  $A_Z$  are also calculated via Fourier space, e.g.  $\partial_X A_Z$  is calculated as the inverse-transform of  $(\partial_X A_Z)^* = ik_X A_Z^*$ , and likewise for higher order derivatives.

In this way, the magnetic field  $(b_x, b_y) = (\partial_Y A_Z, -\partial_X A_Z)$  and its derivative with respect to  $Z$  are determined on a three-dimensional grid. The grid-size in each direction is such that it contains several correlation lengths. The values of  $b_x(X,Y,Z)$  and  $b_y(X,Y,Z)$  for points  $(X,Y,Z)$  in-between the grid-sites are calculated by interpolating the magnetic field components at the nearest grid-sites with 3<sup>rd</sup> order cubic splines. By construction, the magnetic field is periodic in all three directions, and particles leaving the simulation box are re-injected at the plane opposite to the one through which they leave.

## RESULTS

The standard parameter values we use are  $V_{th}/\Omega = 0.3\text{m}$  for the Larmor radius,  $\beta = 10^{-2}$  for the strength of the magnetic perturbations, and for the values of the correlation lengths we assume  $\lambda_X = \lambda_Y = 10^{-2}\text{m}$  and  $\lambda_Z = 1\text{m}$ , so that  $K_m = 1$ ,  $A = 1$ , and  $K_{dr}$  is varied in the range  $[0, 0.6]$ . The stochastic magnetic field is generated on a grid with  $64^3$  grid-points. The diffusivities are determined from  $10^6$  test particles in  $10^3$  different samples of the magnetic field.

For fixed drift Kubo number ( $K_{dr} = 0.2$ ) and for two different magnetic Kubo-numbers, *Fig. 1* shows the radial  $D_{xx}(z)$  and the poloidal  $D_{yy}(z)$  diffusion coefficients for different degrees of anisotropy  $A$ . Basically,  $D_{xx}$  decreases and  $D_{yy}$  increases with increasing  $A$ , whereby this effect is more pronounced the larger  $K_m$  is, i.e. the stronger the magnetic perturbation is.



*Fig. 1: Radial (a) and poloidal (b) running diffusion coefficients for  $K_{dr} = 0.2$  and  $K_m = 3$ , and for different values of the stochastic anisotropy parameter  $A$ . (c) Asymptotic values of the diffusion coefficients as a function of  $A$ , for  $K_{dr} = 0.2$  and two different values of  $K_m$  (0.5 and 3).*

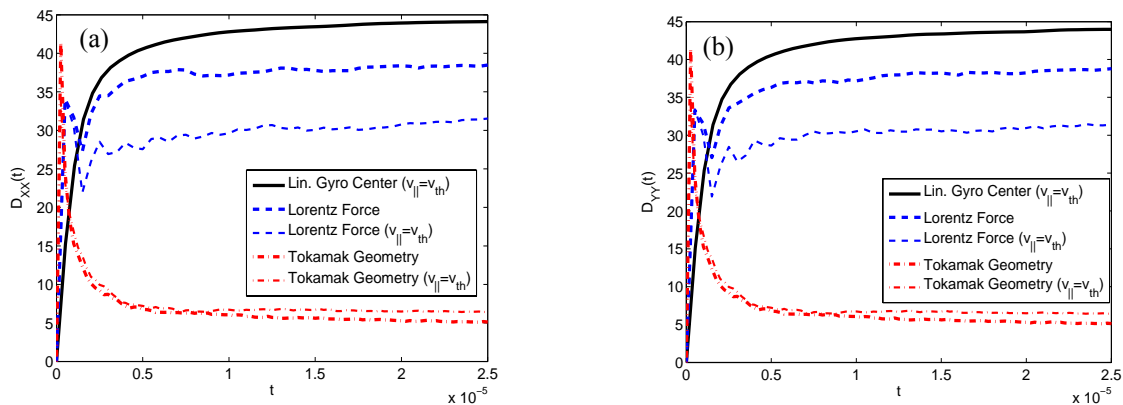
Comparing to the results from the DCT method, we find that the values of the diffusion coefficients coincide within 20% for  $D_{yy}$  in the case  $K_m = 0.5$  and for  $D_{xx}$  in the case  $K_m = 3.0$ , and they also exhibit the same scaling with  $A$ . For  $D_{yy}$  in the case  $K_m = 3.0$  the scaling with  $A$  is the same, the differences in values reach though now 50%, as for  $D_{xx}$  in the case  $K_m = 0.5$ , where moreover the scaling with  $A$  is different. In basically all cases shown so-far, the time needed to reach the asymptotic state is roughly 5 times larger than in the DCT method. A similar agreement between the two methods was found when varying  $K_{dr}$  and keeping the other parameters fixed.

We now investigate how far some of the assumptions we made influence the results. We consider ITER-like conditions and choose  $\text{He}^{2+}$  as test-particles.  $K_{\text{dr}}$  is thus fixed, and we concentrate on the isotropic case ( $\Lambda = 1$ ), with a level of stochastic perturbation  $\beta = 10^{-2}$ .

First, we investigate how accurate the linearised gyro-centre approximation of (2) is. Thereto, we integrate the equations of motion in terms of the Lorentz-force. The two perpendicular components of the initial velocity,  $V_x(0)$  and  $V_y(0)$ , are chosen random with Gaussian distribution that corresponds to the temperature  $T_i$ , and the parallel component  $V_z(0)$  is either random and Gaussian distributed (again with temperature  $T_i$ ), or we let it equal to  $V_{\text{th}} = (3k_B T_i / m_{\text{He}})^{1/2}$ , as in the gyro-centre approximation. *Figure 2* shows the corresponding running diffusion coefficients. With  $V_z(0) = V_{\text{th}}$ , the gyro-centre approximation overestimates the diffusivity by roughly 50%, it is though closer to the case with random  $V_z(0)$ , still overestimating it by now 15%.

Second, we address the question in how far neo-classical effects alter the results presented so-far. Thereto, we use the standard (vacuum) tokamak magnetic field (see [3]) with safety-factor from [4]. Onto the background field, we superpose the stochastic magnetic field (with  $\beta = 10^{-2}$ ) that is numerically generated as before on a 3-D Cartesian grid and transformed to toroidal geometry.

*Figure 2* shows two cases of integrating the Lorentz-force in toroidal geometry, one with random  $V_{\parallel}(0)$  and one with  $V_{\parallel}(0) = V_{\text{th}}$  (with  $V_{\parallel}$  in toroidal geometry corresponding to  $V_z$  in cylindrical geometry), respectively (no drift approximation is applied). They yield very similar results, the approximation  $V_{\parallel} = V_{\text{th}}$  is more valid in toroidal than in cylindrical geometry, the diffusivities are though roughly 7 times smaller than those derived in cylindrical geometry, basically due to neo-classical effects.



*Fig. 2:  $\text{He}^{2+}$  (physical units): Radial (a) and poloidal (b) running diffusion coefficients for  $\beta = 10^{-2}$  and  $\Lambda = 1$ , in cylindrical and toroidal geometry, and with the gyro-centre approximation compared to the integration of the Lorentz force.*

## CONCLUSION

We have shown that the DCT method gives qualitatively satisfying results, and quantitatively it achieves a precision of 50% in the calculation of the diffusion coefficients. Non-linear effects in the gyro-centre approximation, as well as the effects of toroidal geometry, must be taken into account for a quantitatively reliable description of transport.

## REFERENCES

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