

**A General Form of the
Coulomb Scattering Operators
for Monte Carlo Simulations
and a Note on the
Guiding Center Equations in
Different Magnetic Coordinate Conventions**

T.S. CHEN*

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*Permanent address:
Institute of Plasma Physics
Chinese Academy of Sciences, Hefei CHINA

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Abstract

The Monte Carlo Coulomb scattering operators used by A.H. Boozer *et. al.* [1] are extended to a more general form which considers the collisions between a test particle and different Maxwellian background particle species. The reduced angle- and energy-scattering operators in some special situations are also given, e.g., the scattering operators for an energetic test particle and a background plasma consisting of electrons, a major ion species and impurities. As a reference, formulas of various relaxation times which are frequently encountered in Monte Carlo transport simulations are reviewed in the first section of this report. Moreover, in Section III, the guiding center equations for stellarators in two different magnetic coordinate conventions are described. The cgs Gaussian system of units is used throughout.

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1. Relaxation times

1.1 Fokker-Planck equation and Rosenbluth potentials

The general form of charged particle Fokker-Planck equation is:

$$\frac{\partial f}{\partial t} \Big|_c = \sum_b \Gamma_b \left[-\frac{\partial}{\partial \mathbf{v}} \cdot \left(f \frac{\partial h_b}{\partial \mathbf{v}} \right) + \frac{1}{2} \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : \left(f \frac{\partial^2 g_b}{\partial \mathbf{v} \partial \mathbf{v}} \right) \right], \quad (1)$$

where f is the test particle distribution function, \mathbf{v} is the test-particle velocity vector, and h_b and g_b are the Rosenbluth potentials. The subscript b corresponds to the b th species of the background plasma, and

$$\Gamma_b = \frac{4\pi Z^2 Z_b^2 e^4 \ln \Lambda_b}{m^2}, \quad (2)$$

where m is the mass of test particle, Z is the charge number of the test particle, and Z_b is the charge number of the b th background species. The quantity $\ln \Lambda_b$ corresponds to the Coulomb logarithm between the test particle and the b th background species [3]:

$$\Lambda_b \simeq \frac{3}{2} \left(\frac{k^3 T_e^3}{\pi n_e} \right)^{1/2} \frac{1}{Z Z_b e^3},$$

where n_e and T_e are the background electron number density and temperature.

Because of the complexity of the various situations possible, the relaxation times are not very clearly defined parameters. One way [4] to define them is by calculating various velocity moments of Eq. (1) under the following assumptions:

1. The test-particle distribution function is always a delta function in the collisional process, that is

$$f = \delta(\mathbf{v} - \mathbf{u}), \quad (3)$$

where \mathbf{u} is the average velocity of the test particle ensemble.

2. The background charged particle species are in Maxwellian distributions.

The corresponding Rosenbluth potentials are therefore simplified due to the assumption '2':

$$h_b(\mathbf{v}) = \frac{m + m_b}{m_b} \int d\mathbf{v}' f_b(\mathbf{v}') |\mathbf{v} - \mathbf{v}'|^{-1} = h_b(v) = \frac{n_b}{v} \left[\left(1 + \frac{m}{m_b} \right) \Phi(a_b v) \right], \quad (4)$$

$$g_b(\mathbf{v}) = \int d\mathbf{v}' g_b(\mathbf{v}') |\mathbf{v} - \mathbf{v}'| = g_b(v) = n_b \left[\left(v + \frac{1}{2a_b^2 v} \right) \Phi(a_b v) + \frac{\exp(-a_b^2 v^2)}{a_b \sqrt{\pi}} \right], \quad (5)$$

where $\Phi(x)$ is the error function,

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-x^2) dx, \quad (6)$$

and a_b is the reciprocal of the background thermal velocity:

$$a_b = \frac{1}{v_{bth}} = \sqrt{\frac{m_b}{3kT_b}}. \quad (7)$$

The momentum equation of Eq. (1) is

$$\frac{\partial}{\partial t} \int_{\mathbf{v}} \mathbf{w} f d\mathbf{v} = \sum_b \Gamma_b \left[- \int_{\mathbf{v}} \frac{\partial}{\partial \mathbf{v}} \cdot \left(\mathbf{w} f \frac{\partial h_b}{\partial \mathbf{v}} \right) d\mathbf{v} + \frac{1}{2} \int_{\mathbf{v}} \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : \left(\mathbf{w} f \frac{\partial^2 g_b}{\partial \mathbf{v} \partial \mathbf{v}} \right) d\mathbf{v} \right], \quad (8)$$

where \mathbf{w} is the velocity momentum function, and other symbols have their usual meanings.

1.2 Slowing down time

The definition of slowing down time is

$$\tau_s = -u / \frac{\partial u}{\partial t}. \quad (9)$$

Letting $\mathbf{w} = \mathbf{v}$, substituting (3) into (8) and integrating (8) by parts, we find

$$\frac{\partial u}{\partial t} = \sum_b \Gamma_b \frac{\partial h_b(u)}{\partial u}. \quad (10)$$

Substituting $h_b(u)$ from (4) we define

$$\frac{\partial H(u)}{\partial u} = \sum_b \Gamma_b \frac{\partial h_b(u)}{\partial u} = -2n_e \Gamma_e M_e a_e^2 \Psi(a_e u) - 2 \sum_j n_j \Gamma_j M_j a_j^2 \Psi(a_j u), \quad (11)$$

where

$$\begin{aligned} M_e &= 1 + \frac{m}{m_e}, \\ M_j &= 1 + \frac{m}{m_j}, \end{aligned} \quad (12)$$

$$\Psi(x) = \frac{\Phi(x) - x\Phi'(x)}{2x^2}, \quad \text{and} \quad \Phi'(x) = \frac{2}{\sqrt{\pi}} \exp(-x^2). \quad (13)$$

The subscript 'e' corresponds to the background electron species, and 'j' corresponds to the jth background ion species. The summation is taken over all of the background ion species.

From Eqs. (9)–(11) we have

$$\tau_s = \frac{u}{2n_e \Gamma_e M_e a_e^2 \Psi(a_e u) + 2 \sum_j n_j \Gamma_j M_j a_j^2 \Psi(a_j u)}. \quad (14)$$

In the usual neutral beam injection case, $u_{j\text{th}} \ll u \ll u_{e\text{th}}$, then

$$\begin{aligned} \Psi(a_e u) &\simeq \frac{2}{3} \frac{a_e u}{\sqrt{\pi}} \quad \left(\text{as } x \rightarrow 0, \quad \Psi(x) \rightarrow \frac{2}{3} \frac{x}{\sqrt{\pi}} \right), \\ \Psi(a_j u) &\simeq \frac{1}{2(a_j u)^2} \quad \left(\text{as } x \rightarrow \infty, \quad \Psi(x) \rightarrow 2 \frac{1}{x^2} \right). \end{aligned} \quad (15)$$

Recalling Eqs. (2) and (7) gives

$$\tau_s \simeq \frac{m^2}{4\pi Z^2 e^4 n \ln \Lambda} : \left[\frac{\langle Z \rangle + A[Z]}{u^3} + \frac{4}{3\sqrt{\pi}} M_e \left(\frac{m_e}{3kT_e} \right)^{3/2} \right], \quad (16)$$

where two kinds of effective Z for the background plasma ions have been defined as:

$$[Z] \equiv \sum_j \frac{Z_j^2 n_j \ln \Lambda_j}{A_j n \ln \Lambda}, \quad (17)$$

$$\langle Z \rangle \equiv \sum_j \frac{Z_j^2 n_j \ln \Lambda_j}{n \ln \Lambda}, \quad (18)$$

where $n = n_e$ (electron number density), $\ln \Lambda = \ln \Lambda_e$, and $A = m/m_p$, $A_j = m_j/m_p$, with m_p the proton mass.

1.3 Deflection time

The definition of 90° pitch angle deflection time is

$$\tau_D \equiv u^2 / \frac{\partial u_{\perp}^2}{\partial t}. \quad (19)$$

Letting $\mathbf{w} = \mathbf{v} \cdot \mathbf{v}$, substituting f from Eq. (3), then Eq. (8) gives

$$\frac{\partial}{\partial t}(\mathbf{u} \cdot \mathbf{u}) = \sum_b \Gamma_b \left[2\mathbf{u} \cdot \frac{\partial h_b}{\partial \mathbf{u}} + \frac{\partial}{\partial \mathbf{u}} \cdot \frac{\partial g_b}{\partial \mathbf{u}} \right]. \quad (20)$$

Suppose that at $t = 0$, $\mathbf{u} = iu_x$, then Eq. (20) is reduced to

$$\frac{\partial u^2}{\partial t} = \sum_b \Gamma_b \left[2u_x \frac{\partial h_b}{\partial u_x} + \frac{\partial^2 g_b}{\partial u_x^2} + \frac{\partial^2 g_b}{\partial u_y^2} + \frac{\partial^2 g_b}{\partial u_z^2} \right]. \quad (21)$$

Obviously, letting $\mathbf{w} = iu_x \cdot iu_x$, Eq. (8) gives

$$\frac{\partial u_x^2}{\partial t} = \sum_b \Gamma_b \left[2u_x \frac{\partial h_b}{\partial u_x} + \frac{\partial^2 g_b}{\partial u_x^2} \right]. \quad (22)$$

If we assume that the initial direction of the test particle is parallel to the magnetic field, and note furthermore that for a weak dispersion test beam $\mathbf{u} = iu_x = u_{\parallel}$ is true during a suitably long relaxation process, Eq. (22) becomes

$$\frac{\partial u_{\parallel}^2}{\partial t} = \sum_b \Gamma_b \left[2u_{\parallel} \frac{\partial h_b}{\partial u_{\parallel}} + \frac{\partial^2 g_b}{\partial u_{\parallel}^2} \right]. \quad (23)$$

For the perpendicular component, considering Eqs. (21), (22), and (23),

$$\frac{\partial u_{\perp}^2}{\partial t} = \frac{\partial u_y^2}{\partial t} + \frac{\partial u_z^2}{\partial t} = \sum_b \Gamma_b \left[\frac{\partial^2 g_b}{\partial u_y^2} + \frac{\partial^2 g_b}{\partial u_z^2} \right] = \frac{\partial^2 G(u)}{\partial u_y^2} + \frac{\partial^2 G(u)}{\partial u_z^2}, \quad (24)$$

thus

$$\tau_D = u^2 : \left[\frac{\partial^2 G(u)}{\partial u_y^2} + \frac{\partial^2 G(u)}{\partial u_z^2} \right], \quad (25)$$

where, from Eq. (5), we have defined

$$\frac{\partial G(u)}{\partial u} \equiv \sum_b \Gamma_b \frac{\partial g_b}{\partial u} = n\Gamma_e [\Phi(a_e u) - \Psi(a_e u)] + \sum_j \Gamma_j n_j [\Phi(a_j u) - \Psi(a_j u)], \quad (26)$$

and thus

$$\frac{\partial G(u)}{\partial u_y} = \frac{\partial G(u)}{\partial u} \frac{\partial u}{\partial u_y} = \frac{u_y}{u} \frac{\partial G(u)}{\partial u}.$$

Note that at $t = 0$, $u_y = u_z = 0$, then

$$\frac{\partial^2 G(u)}{\partial u_y^2} = \frac{n}{u} \Gamma_e [\Phi(a_e u) - \Psi(a_e u)] + \sum_j \frac{n_j}{u} \Gamma_j [\Phi(a_j u) - \Psi(a_j u)],$$

$$\frac{\partial^2 G(u)}{\partial u_z^2} = \frac{\partial^2 G(u)}{\partial u_y^2},$$

and

$$\frac{\partial u_{\perp}^2}{\partial t} = \frac{2n}{u} \Gamma_e [\Phi(a_e u) - \Psi(a_e u)] + 2 \sum_j \frac{n_j}{u} \Gamma_j [\Phi(a_j u) - \Psi(a_j u)]. \quad (27)$$

Therefore

$$\tau_D = \frac{u^3}{2n\Gamma_e [\Phi(a_e u) - \Psi(a_e u)] + 2 \sum_j n_j \Gamma_j [\Phi(a_j u) - \Psi(a_j u)]}. \quad (28)$$

For the usual NBI case

$$\Phi(a_e u) \simeq \frac{2a_e u}{\sqrt{\pi}} \quad (a_e u \ll 1),$$

$$\Phi(a_j u) \simeq 1 \quad (a_j u \gg 1), \quad (29)$$

and, recalling Eq. (15), Eq. (28) reduces to

$$\tau_D \simeq \frac{u^3}{2n\Gamma} : \left(\frac{4a_e u}{3\sqrt{\pi}} + \langle Z \rangle - \frac{A}{a_i^2 u^2} [Z] \right), \quad (30)$$

where $\langle Z \rangle$ and $[Z]$ are defined by Eqs. (18) and (17), and

$$2n\Gamma = \frac{8\pi Z^2 n e^4 \ln \Lambda}{m^2}. \quad (31)$$

More approximately

$$\tau_D \simeq \frac{A^2 m_p^2 u^3}{8\pi Z^2 \langle Z \rangle e^4 n \ln \Lambda}. \quad (32)$$

In the situation that the test particles collide with an ideal background plasma (i.e. electrons plus a single ion species), Eq. (28) reduced to

$$\tau_D = \frac{u^3}{2n\Gamma [\Phi(a_e u) - \Psi(a_e u)] + 2n_i \Gamma_i [\Phi(a_i u) - \Psi(a_i u)]} \quad (33)$$

and the corresponding deflection frequency is

$$\nu_D = \frac{1}{\tau_D} = \nu_{D_e} + \nu_{D_i},$$

where ν_{D_e} is the deflection frequency of test particle on background electrons,

$$\nu_{D_e} = \frac{3}{2} \sqrt{\pi} \frac{Z^2}{Z_i} \left(\frac{m_e}{m} \right)^2 \nu_{B_e} \frac{\Phi(x_e) - \Psi(x_e)}{x_e^3}, \quad (34)$$

and ν_{D_i} is the deflection frequency of test particle on background ions,

$$\nu_{D_i} = 3 \sqrt{\frac{\pi}{2}} \frac{Z^2}{Z_i^2} \left(\frac{m_i}{m} \right)^2 \nu_{B_i} \frac{\Phi(x_i) - \Psi(x_i)}{x_i^3}. \quad (35)$$

Here

$$x_e = a_e u = u \sqrt{\frac{m_e}{3kT_e}}, \quad (36)$$

$$x_i = a_i u = u \sqrt{\frac{m_i}{3kT_i}}, \quad (37)$$

$$\nu_{B_e} = \frac{4}{3} \sqrt{\frac{2\pi}{m_e}} \frac{Z_i^2 e^4 n_i \ln \Lambda}{\left(\frac{3}{2} kT_e\right)^{\frac{3}{2}}}, \quad (38)$$

and

$$\nu_{B_i} = \frac{4}{3} \sqrt{\frac{\pi}{m_i}} \frac{Z_i^3 e^4 n \ln \Lambda_i}{\left(\frac{3}{2} kT_i\right)^{\frac{3}{2}}}, \quad (39)$$

ν_{B_e} and ν_{B_i} are Braginskii electron and ion collision frequencies respectively [6]. The Braginskii collision frequencies ν_{B_e} and ν_{B_i} can also be written:

$$\nu_{B_e} = \frac{\ln \Lambda}{3.5 \times 10^5} \frac{Z_i n}{T_e^{\frac{3}{2}}} \quad (40)$$

and

$$\nu_{B_i} = \frac{\ln \Lambda}{3 \times 10^7} \sqrt{\frac{2}{A}} \frac{z_i^3 n}{T_i^{\frac{3}{2}}}, \quad (41)$$

where T_e and T_i are in units of electron volts.

1.4 Energy relaxation time

We define

$$\tau_W \equiv -W / \frac{\partial W}{\partial t}, \quad (42)$$

where $W = \frac{1}{2}mu^2$ is the kinetic energy of a test particle.

$$\frac{\partial W}{\partial t} = \frac{1}{2}m \frac{\partial u^2}{\partial t} = \frac{1}{2}m \left(\frac{\partial u_{\parallel}^2}{\partial t} + \frac{\partial u_{\perp}^2}{\partial t} \right), \quad (43)$$

where

$$\frac{\partial u_{\parallel}^2}{\partial t} = \sum_b \Gamma_b \left[2u_{\parallel} \frac{\partial h_b}{\partial u_{\parallel}} + \frac{\partial^2 g_b}{\partial u_{\parallel}^2} \right]. \quad (44)$$

Recalling Eq. (11) and noting that at $t = 0$, $u_{\parallel} = u$, $u_{\perp} = 0$, we have

$$\sum_b \Gamma_b 2u_{\parallel} \frac{\partial h_b}{\partial u_{\parallel}} = 2u \sum_b \Gamma_b \frac{\partial h_b}{\partial u} \frac{\partial u}{\partial u_{\parallel}} = 2u \frac{\partial H(u)}{\partial u} \quad (45)$$

and, recalling (26),

$$\sum_b \Gamma_b \frac{\partial^2 g_b}{\partial u_{\parallel}^2} = \frac{\partial}{\partial u_{\parallel}} \left[\frac{\partial G(u)}{\partial u} \frac{u_{\parallel}}{u} \right] = \frac{2n\Gamma}{u} \Psi(a_e u) + \frac{2}{u} \sum_j n_j \Gamma_j \Psi(a_j u). \quad (46)$$

Note that the relation

$$\Psi'(x) = \frac{d}{dx} \left(\frac{\Phi(x) - x\Phi'(x)}{2x^2} \right) = \Phi'(x) - \frac{2}{x} \Psi(x) \quad (47)$$

has been used to get (46).

From Eqs. (45), (46), and (27) we have

$$\frac{\partial u_{\parallel}^2}{\partial t} + \frac{\partial u_{\perp}^2}{\partial t} = \frac{2n\Gamma}{u} [\Phi(a_e u) - 2M_e a_e^2 u^2 \Psi(a_e u)] + \frac{2}{u} \sum_j n_j \Gamma_j [\Phi(a_j u) - 2M_j a_j^2 u^2 \Psi(a_j u)]$$

or, by recalling Eqs. (12) and (13),

$$\begin{aligned} \frac{\partial u_{\parallel}^2}{\partial t} + \frac{\partial u_{\perp}^2}{\partial t} &= 4n\Gamma a_e \left[\frac{1}{2} \Phi'(a_e u) - \frac{m}{m_e} a_e u \Psi(a_e u) \right] \\ &\quad + 4 \sum_j n_j \Gamma_j a_j \left[\frac{1}{2} \Phi'(a_j u) - \frac{m}{m_j} a_j u \Psi(a_j u) \right]. \end{aligned} \quad (48)$$

We thus obtain

$$\tau_W = \frac{-u^2/4}{n\Gamma a_e \left[\frac{1}{2} \Phi'(a_e u) - \frac{m}{m_e} a_e u \Psi(a_e u) \right] + \sum_j n_j \Gamma_j a_j \left[\frac{1}{2} \Phi'(a_j u) - \frac{m}{m_j} a_j u \Psi(a_j u) \right]}. \quad (49)$$

The corresponding energy relaxation frequency is

$$\nu_W = \frac{1}{\tau_W} = \nu_{W_e} + \nu_{W_i},$$

where ν_{W_e} is the energy relaxation frequency of test particles on background electrons,

$$\nu_{W_e} = \frac{16\pi Z^2 e^4 n \ln \Lambda}{m^2} a_e^3 \frac{\frac{m}{m_e} x_e \Psi(x_e) - \frac{1}{2} \Phi'(x_e)}{x_e^2}, \quad (50)$$

ν_{W_i} is the energy relaxation frequency of test particles on background ion species,

$$\nu_{W_i} = \frac{16\pi Z^2 e^4}{m^2} \sum_j a_j^3 Z_j^2 n_j \ln \Lambda_j \frac{\frac{m}{m_j} x_j \Psi(x_j) - \frac{1}{2} \Phi'(x_j)}{x_j^2}, \quad (51)$$

and x_e, x_j, a_e, a_j have been defined by (36) and (37).

For the usual NBI case, the $\frac{1}{2} \Phi'(x)$ terms may be ignored, Eqs. (50) and (51) reduce to

$$\nu_{W_e} = \frac{16\pi Z^2 e^4 n \ln \Lambda}{A(3kT_e)^{\frac{3}{2}}} \frac{\sqrt{m_e}}{m_p} \frac{\Psi(x_e)}{x_e} \quad (52)$$

and

$$\nu_{W_i} = \frac{16\pi Z^2 e^4}{A(3kT_i)^{\frac{3}{2}}} \sum_j Z_j^2 n_j \ln \Lambda_j \frac{\sqrt{m_j}}{m_p} \frac{\Psi(x_j)}{x_j}. \quad (53)$$

In Eq. (51) we have supposed that

$$a_j = \sqrt{\frac{m_j}{3kT_i}} \quad (\text{if } T_j = T_i), \quad (54)$$

where the index i corresponds to the major species of the background ions.

More approximately (considering Eq. (15)),

$$\nu_{W_e} \simeq \frac{16\pi Z^2 e^4 n \ln \Lambda}{A(3kT_e)^{\frac{3}{2}}} \frac{\sqrt{m_e}}{m_p} \frac{2}{3\sqrt{\pi}} \quad (55)$$

and

$$\nu_{W_i} \simeq \frac{16\pi Z^2 e^4 n \ln \Lambda}{A(3kT_i)^{\frac{3}{2}}} \sum_j \frac{Z_j^2 n_j \ln \Lambda_j}{n \ln \Lambda} \frac{\sqrt{m_j}}{m_p} \frac{1}{2x_j^3} = \frac{8\pi Z^2 [Z] e^4 n \ln \Lambda}{Am_p^2 u^3}. \quad (56)$$

The effective $[Z]$ has been defined in Eq. (17).

In case of a single background ion species, Eqs. (52) and (53) may be written as

$$\nu_{W_e} = 3\sqrt{\pi} \nu_{B_e} \frac{m_e}{m} \frac{Z^2}{Z_i} \frac{\Psi(x_e)}{x_e} \quad (57)$$

and

$$\nu_{W_i} = 3\sqrt{2\pi} \nu_{B_i} \frac{m_i}{m} \frac{Z^2}{Z_i^2} \frac{\Psi(x_i)}{x_i}, \quad (58)$$

where ν_{B_e} and ν_{B_i} have been defined in Eqs. (38) and (40).

2. Monte Carlo scattering operators

The Lorentz scattering operators and the equivalent Monte Carlo scattering operators used by A.H. Boozer *et. al.* [1] are only suitable for like particle (ion-ion) interactions. In this section we extend these operators to a general for which can consider the interactions between test particles and different field particle species (i.e. with different masses, charge numbers, temperatures or energies). The reduced equivalent Monte Carlo operators under some special situations are given.

2.1 General form of the Lorentz scattering operators

We use the azimuthally symmetric Fokker-Planck collision term in spherical polar velocity space (u, λ, ϕ) [2] to derive the extended Lorentz scattering operators.

Since the background plasma is assumed to be a Maxwellian distribution with constant temperature and number densities (i.e. the Lorentz approximation), and the Rosenbluth potentials are simply given by Eqs. (4) and (5), the original Fokker-Planck collision term therefore is reduced to

$$\begin{aligned} \left. \frac{\partial f}{\partial t} \right|_c = \sum_b \Gamma_b \left\{ \frac{1}{2u^2} \frac{\partial^2}{\partial u^2} \left(u^2 \frac{\partial^2 g_b}{\partial u^2} f \right) - \frac{1}{u^2} \frac{\partial}{\partial u} \left[f \left(u^2 \frac{\partial h_b}{\partial u} + \frac{\partial g_b}{\partial u} \right) \right] \right. \\ \left. + \frac{1}{2u^3} \frac{\partial g_b}{\partial u} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial f}{\partial \lambda} \right\}, \end{aligned} \quad (59)$$

where $f = f(t, u, \lambda)$ is the test particle distribution function, and $\lambda = u_{\parallel}/u = \cos \theta$, where θ is the angle between magnetic field \mathbf{B} and test particle velocity vector \mathbf{u} .

Recalling (11) and (26), Eq. (59) may be written as

$$\begin{aligned} \left. \frac{\partial f}{\partial t} \right|_c = \frac{1}{2u^2} \frac{\partial^2}{\partial u^2} \left(u^2 \frac{\partial^2 G}{\partial u^2} f \right) - \frac{1}{u^2} \frac{\partial}{\partial u} \left[f \left(u^2 \frac{\partial H}{\partial u} + \frac{\partial G}{\partial u} \right) \right] \\ + \frac{1}{2u^3} \frac{\partial G}{\partial u} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial f}{\partial \lambda}, \end{aligned} \quad (60)$$

where

$$\frac{\partial^2 G}{\partial u^2} = \frac{2n}{u} \Gamma \Psi(a_e u) + \frac{2}{u} \sum_j n_j \Gamma_j \Psi(a_j u). \quad (61)$$

After some calculation, Eq. (60) may be further simplified to

$$\begin{aligned} \left. \frac{\partial f}{\partial t} \right|_c = \frac{1}{u^2} \frac{\partial}{\partial u} \left\{ u^2 \frac{\partial}{\partial u} \left[n a_e^2 \Gamma \frac{m}{m_e} \Psi(x_e) + \sum_j n_j a_j^2 \Gamma_j \frac{m}{m_j} \Psi(x_j) \right] f \right\} \\ + \frac{1}{2u^2} \frac{\partial}{\partial u} \left[u^2 \frac{\partial^2 G}{\partial u^2} \frac{\partial f}{\partial u} \right] + \frac{1}{2u^3} \frac{\partial G}{\partial u} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial f}{\partial \lambda}, \end{aligned} \quad (62)$$

where x_e, x_j have been defined in (36) and (37).

For the first right term of Eq. (62) we get

$$\begin{aligned}
& 2na_e^2\Gamma\frac{m}{m_e}\Psi(x_e) + 2\sum_j n_j a_j^2\Gamma_j\frac{m}{m_j}\Psi(x_j) \\
&= u\frac{8\pi Z^2 e^4 n \ln \Lambda}{A}\frac{a_e^3}{m_p m_e}\frac{\Psi(x_e)}{x_e} + u\frac{8\pi Z^2 e^4}{A}\sum_j Z_j^2 n_j \ln \Lambda_j\frac{a_j^3}{m_p m_j}\frac{\Psi(x_j)}{x_j} \\
&= u\frac{8\pi Z^2 e^4 n \ln \Lambda}{A(3kT_e)^{\frac{3}{2}}}\frac{\sqrt{m_e}}{m_p}\frac{\Psi(x_e)}{x_e} + u\frac{8\pi Z^2 e^4}{A(3kT_i)^{\frac{3}{2}}}\sum_j Z_j^2 n_j \ln \Lambda_j\frac{\sqrt{m_j}}{m_p}\frac{\Psi(x_j)}{x_j} \\
&= u\nu_{E_e} + u\nu_{E_i} = u\nu_E,
\end{aligned} \tag{63}$$

where

$$\nu_{E_e} = \frac{8\pi Z^2 e^4 n \ln \Lambda}{A(3kT_e)^{\frac{3}{2}}}\frac{\sqrt{m_e}}{m_p}\frac{\Psi(x_e)}{x_e}, \tag{64}$$

and

$$\nu_{E_i} = \frac{8\pi Z^2 e^4}{A(3kT_i)^{\frac{3}{2}}}\sum_j Z_j^2 n_j \ln \Lambda_j\frac{\sqrt{m_j}}{m_p}\frac{\Psi(x_j)}{x_j}. \tag{65}$$

Here ν_{E_e} and ν_{E_i} are the general forms of the energy relaxation frequencies derived from the generalized Lorentz operator. Note that, comparing with the previously defined energy relaxation frequency (Eqs. (52) and (53)), $\nu_E \simeq \frac{1}{2}\nu_W$.

For the second right term of Eq. (62), from (61)

$$\begin{aligned}
\frac{\partial^2 G}{\partial u^2} &= \frac{8\pi Z^2 e^4 n \ln \Lambda}{m^2}a_e\frac{\Psi(x_e)}{x_e} + \frac{8\pi Z^2 e^4}{m^2}\sum_j Z_j^2 n_j \ln \Lambda_j a_j\frac{\Psi(x_j)}{x_j} \\
&= \frac{8\pi Z^2 e^4 n \ln \Lambda}{A(3kT_e)^{\frac{3}{2}}}\frac{\sqrt{m_e}}{m_p}\frac{\Psi(x_e)}{x_e}\frac{3kT_e}{m} + \frac{8\pi Z^2 e^4}{A(3kT_i)^{\frac{3}{2}}}\sum_j Z_j^2 n_j \ln \Lambda_j\frac{\sqrt{m_j}}{m_p}\frac{\Psi(x_j)}{x_j}\frac{3kT_i}{m}.
\end{aligned}$$

Comparing with Eqs. (64) and (65) we have

$$\frac{\partial^2 G}{\partial u^2} = \nu_{E_e}\frac{3kT_e}{m} + \nu_{E_i}\frac{3kT_i}{m}$$

and then the second right term of Eq. (62) reads

$$\frac{1}{2u^2}\frac{\partial}{\partial u}\left[u^2\frac{\partial^2 G}{\partial u^2}\frac{\partial f}{\partial u}\right] = \frac{1}{u^2}\frac{\partial}{\partial u}\left[u^2\left(\nu_{E_e}\frac{3kT_e}{2m} + \nu_{E_i}\frac{3kT_i}{2m}\right)\frac{\partial f}{\partial u}\right]. \tag{66}$$

Hereafter, we shall write $\frac{3}{2}kT$ simply as T , so that T should be understood to be in units of energy (ergs in cgs unit system).

For the third right term of Eq. (62), recalling Eq. (26), we get

$$\frac{\partial G}{\partial u} = \frac{4\pi Z^2 e^4 n \ln \Lambda}{m^2} \left\{ \Phi(x_e) - \Psi(x_e) + \sum_j \frac{Z_j^2 n_j \ln \Lambda_j}{n \ln \Lambda} [\Phi(x_j) - \Psi(x_j)] \right\} = u^3 \nu_d, \quad (67)$$

where

$$\nu_d = \frac{4\pi Z^2 e^4 n \ln \Lambda}{m^2 u^3} \left\{ \Phi(x_e) - \Psi(x_e) + \sum_j \frac{Z_j^2 n_j \ln \Lambda_j}{n \ln \Lambda} [\Phi(x_j) - \Psi(x_j)] \right\}. \quad (68)$$

Here ν_d is the general form of the test particle deflection frequency derived from the generalized Lorentz operator. Note that, comparing with the previously defined deflection time (Eq. (28)), $\nu_d = \frac{1}{2} \nu_D$.

Substituting (63), (66), and (67) into (62), the generalized Lorentz collision operator now is written as

$$\begin{aligned} \left. \frac{\partial f}{\partial t} \right|_c &= \frac{\nu_d}{2} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial f}{\partial \lambda} \\ &+ \frac{1}{u^2} \frac{\partial}{\partial u} [u^2 (\nu_E u f)] + \frac{1}{u^2} \frac{\partial}{\partial u} \left[u^2 \left(\nu_{E_e} \frac{T_e}{m} + \nu_{E_i} \frac{T_i}{m} \right) \frac{\partial f}{\partial u} \right], \end{aligned} \quad (69)$$

where the generalized Lorentz angle scattering operator is

$$\frac{\partial f}{\partial t} = \frac{\nu_d}{2} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial f}{\partial \lambda}, \quad (70)$$

which is the same as that used by Boozer *et. al.* [1] except that the 90° deflection frequency ν_d here is extended to be able to consider the collisions between test particle and various field species (Eq. (68)).

The generalized Lorentz energy scattering operator is

$$\frac{\partial f}{\partial t} = \frac{1}{u^2} \frac{\partial}{\partial u} [u^2 (\nu_E u f)] + \frac{1}{u^2} \frac{\partial}{\partial u} \left[u^2 \left(\nu_{E_e} \frac{T_e}{m} + \nu_{E_i} \frac{T_i}{m} \right) \frac{\partial f}{\partial u} \right], \quad (71)$$

which is an extended form of that used by Boozer *et. al.* [1], and thus can describe the interactions between test particle and various field species.

2.2 The equivalent Monte Carlo scattering operators

(i). The equivalent angle scattering operator:

This is the same as that used by Boozer *et. al.* [1],

$$\lambda_n = \lambda_0(1 - \nu_d \tau) \pm \sqrt{(1 - \lambda_0^2)\nu_d \tau} \quad (72)$$

except that here ν_d considers collisions between the test particle and various field species (Eq. (68)).

(ii). The equivalent energy scattering operator:

Completely following Boozer *et. al.* let

$$\langle E \rangle = \int_0^\infty \frac{1}{2} m u^2 f(t, u) 4\pi u^2 du \quad (73)$$

and

$$\langle E^2 \rangle = \int_0^\infty \left(\frac{1}{2} m u^2 \right)^2 f(t, u) 4\pi u^2 du \quad (74)$$

Then, substituting (71) into (73) and (74), we get the following relations after integration by parts:

$$\begin{aligned} \frac{d\langle E \rangle}{dt} &= \int_0^\infty \frac{1}{2} m u^2 \frac{\partial f}{\partial t} 4\pi u^2 du \\ &= -2\nu_e \langle E \rangle + 3\nu_{E_e} T_e + 2\langle E \rangle \frac{d\nu_{E_e}}{dE} T_e + 3\nu_{E_i} T_i + 2\langle E \rangle \frac{d\nu_{E_i}}{dE} T_i \end{aligned} \quad (75)$$

and

$$\begin{aligned} \frac{d\langle E^2 \rangle}{dt} &= \int_0^\infty \left(\frac{1}{2} m u^2 \right)^2 \frac{\partial f}{\partial t} 4\pi u^2 du \\ &= -4\nu_E \langle E^2 \rangle + 10\nu_{E_e} \langle E \rangle + 4\langle E^2 \rangle T_e \frac{d\nu_{E_e}}{dE} + 10\nu_{E_i} \langle E \rangle + 4\langle E^2 \rangle T_i \frac{d\nu_{E_i}}{dE}. \end{aligned} \quad (76)$$

The time derivative of the standard deviation of $f(t, u)$ in energy space is

$$\frac{d\sigma^2}{dt} = \frac{d\langle E^2 \rangle}{dt} - \frac{d\langle E \rangle^2}{dt} = \frac{d\langle E^2 \rangle}{dt} - 2\langle E \rangle \frac{d\langle E \rangle}{dt}. \quad (77)$$

Substituting Eqs. (75) and (76) into Eq. (77), and supposing that at $t = 0$, $f(0, u)$ is a delta function about $u = u_0$ ($E = E_0$) and with quite small dispersion within a short time duration τ , this leads to $\langle E \rangle \simeq E_0$, $\langle E^2 \rangle \simeq E_0^2$ and gives

$$\frac{d\sigma^2}{dt} = 4\nu_{E_e} E_0 T_e + 4\nu_{E_i} E_0 T_i$$

implying

$$\sigma = 2\sqrt{E_0(\nu_{E_e}T_e + \nu_{E_i}T_i)\tau} \quad (78)$$

as $\tau \rightarrow 0$.

The center of the energy deviation at $t = \tau$ ($\tau \rightarrow 0$) is expected by Eq. (75):

$$E = E_0 - 2\nu_{E_e}\tau \left[E_0 - \left(\frac{3}{2} + \frac{E_0}{\nu_{E_e}} \frac{d\nu_{E_e}}{dE} \right) T_e \right] - 2\nu_{E_i}\tau \left[E_0 - \left(\frac{3}{2} + \frac{E_0}{\nu_{E_i}} \frac{d\nu_{E_i}}{dE} \right) T_i \right]. \quad (79)$$

After considering the fluctuation we find the equivalent Monte Carlo energy scattering operator for the generalized Lorentz energy scattering operator (Eq. (71)), which reduces to Boozer's operator if there are only like particle interactions. It reads

$$E_n = E_0 - 2\nu_{E_e}\tau \left[E_0 - \left(\frac{3}{2} + \frac{E_0}{\nu_{E_e}} \frac{d\nu_{E_e}}{dE} \right) T_e \right] - 2\nu_{E_i}\tau \left[E_0 - \left(\frac{3}{2} + \frac{E_0}{\nu_{E_i}} \frac{d\nu_{E_i}}{dE} \right) T_i \right] \pm 2\sqrt{E_0(\nu_{E_e}T_e + \nu_{E_i}T_i)\tau}, \quad (80)$$

where E_0 is the old value of the energy E ($= \frac{1}{2}mu^2$) at $t = t_0$, and E_n is the new value of E at $t = t_0 + \tau$. The symbol \pm means the sign is to be chosen randomly, but with equal probability for plus and minus.

Eq. (80) should be furthermore written to be convenient for computation. Recalling (64), the factor

$$\frac{E}{\nu_{E_e}} \frac{d\nu_{E_e}}{dE} = \frac{1}{\nu_{E_e}} \frac{8\pi Z^2 e^4 n \ln \Lambda}{A(2T_e)^{\frac{3}{2}}} \frac{\sqrt{m_e}}{m_p} x_e^2 \frac{d}{dx_e^2} \left(\frac{\Psi(x_e)}{x_e} \right), \quad (81)$$

where

$$\frac{d}{dx^2} \left(\frac{\Psi(x)}{x} \right) = \frac{1}{x^2} \left[\frac{\exp(-x^2)}{\sqrt{\pi}} - \frac{3}{2} \frac{\Psi(x)}{x} \right], \quad (82)$$

we have

$$\left(\frac{3}{2} + \frac{E_0}{\nu_{E_e}} \frac{d\nu_{E_e}}{dE} \right) T_e = \frac{x_e}{\sqrt{\pi}} \frac{\exp(-x_e^2)}{\Psi(x_e)} T_e. \quad (83)$$

Similarly for the test particle-ion interaction term

$$\left(\frac{3}{2} + \frac{E_0}{\nu_{E_i}} \frac{d\nu_{E_i}}{dE} \right) T_i = \left[\sum_j Z_j^2 n_j \ln \Lambda_j A_j^{\frac{1}{2}} \frac{\exp(-x_j^2)}{\sqrt{\pi}} : \left(\sum_j Z_j^2 n_j \ln \Lambda_j A_j^{\frac{1}{2}} \frac{\Psi(x_j)}{x_j} \right) \right] T_i. \quad (84)$$

Substituting Eqs. (83) and (84) into Eq. (80), we obtain the computing form of the generalized Monte Carlo energy operator:

$$x_n^2 = x_0^2 - 2\nu_{E_e}\tau \left[x_0^2 - \frac{\alpha}{\sqrt{\pi}} \frac{cx_0 \exp(-c^2x_0^2)}{\Psi(cx_0)} \frac{T_e}{T_i} \right]$$

$$\begin{aligned}
& -2\nu_{E_i}\tau \left[x_0^2 - \alpha \left(\sum_j Z_j^2 n_j \ln \Lambda_j A_j^{\frac{1}{2}} \frac{\exp(-x_j^2)}{\sqrt{\pi}} \right) : \left(\sum_j Z_j^2 n_j \ln \Lambda_j A_j^{\frac{1}{2}} \frac{\Psi(x_j)}{x_j} \right) \right] \\
& \pm 2x_0 \sqrt{\alpha \left(\nu_{E_i} + \nu_{E_e} \frac{T_e}{T_i} \right) \tau}, \tag{85}
\end{aligned}$$

where

$$\alpha = \frac{m_i}{m}, \quad c = \sqrt{\frac{m_e T_i}{m_i T_e}} = \frac{u_{ith}}{u_{eth}}, \quad A_j = \frac{m_j}{m_p},$$

and

$$x_j = a_j u = \frac{u}{u_{jth}} = \frac{u}{\sqrt{2T_i/m_j}} \quad \text{and} \quad x_i = a_i u = \frac{u}{u_{ith}} = \frac{u}{\sqrt{2T_i/m_i}}.$$

Here m is the mass of test particle, m_i is the ion mass of the major field species, and m_j is the ion mass of the j th field species, x_0 is the old value of x_i at $t = t_0$, and x_n is the new value of x_i at $t = t_0 + \tau$. The energy relaxation frequencies ν_{E_e} and ν_{E_i} have been shown in Eqs. (64) and (65). Other symbols have their usual meanings.

2.3 The reduced Monte Carlo scattering operators

The generalized operators may be reduced to be more simple and useful forms in several special situations.

(i). Test ions colliding with like ions:

The angle scattering operator is as shown in (72), but with the reduced deflection frequency (from Eq. (68)),

$$\nu_d = \frac{4\pi Z^3 e^4 n \ln \Lambda_i}{m^2 u^3} [\Phi(x) - \Psi(x)] = \frac{3}{2} \sqrt{\frac{\pi}{2}} \nu_{B_i} \frac{\Phi(x) - \Psi(x)}{x^3}, \quad (86)$$

where ν_{B_i} is the ion Braginskii frequency (Eq. (40)), and $x = x_i$.

The energy scattering operator reduces to

$$x_n^2 = x_0^2 - 2\nu_E \tau \left[x_0^2 - \frac{x_0}{\sqrt{\pi}} \frac{\exp(-x_0^2)}{\Psi(x_0)} \right] \pm 2x_0 \sqrt{\nu_E \tau}, \quad (87)$$

where, from Eq. (65), the energy relaxation frequency ν_E is now

$$\nu_E = \frac{8\pi Z^3 e^4 n \ln \Lambda_i}{A(2T)^{\frac{3}{2}}} \frac{\sqrt{m_i}}{m_p} \frac{\Psi(x)}{x} = 3 \sqrt{\frac{\pi}{2}} \nu_{B_i} \frac{\Psi(x)}{x}. \quad (88)$$

These reduced operators are the same as those used by Boozer *et. al.* in the transport calculations of Ref. [1].

(ii). Test particles ($E = \frac{1}{2}mu^2$) colliding with an ideal field plasma (electron species + single ion species):

The angle scattering operator is the same as in Eq. (72), but with the reduced deflection frequency

$$\nu_d = \nu_{d_e} + \nu_{d_i},$$

where

$$\nu_{d_e} = \frac{3}{4} \sqrt{\pi} \frac{Z^2}{Z_i} \left(\frac{m_e}{m} \right)^2 \nu_{B_e} \frac{\Phi(x_e) - \Psi(x_e)}{x_e^3} \quad (89)$$

and

$$\nu_{d_i} = \frac{3}{2} \sqrt{\frac{\pi}{2}} \frac{Z^2}{Z_i^2} \left(\frac{m_i}{m} \right)^2 \nu_{B_i} \frac{\Phi(x_i) - \Psi(x_i)}{x_i^3}. \quad (90)$$

The energy scattering operator becomes

$$x_n^2 = x_0^2 - 2\nu_{E_e} \tau \left[x_0^2 - \frac{\alpha}{\sqrt{\pi}} \frac{cx_0 \exp(-c^2 x_0^2) T_e}{\Psi(cx_0) T_i} \right] - 2\nu_{E_i} \tau \left[x_0^2 - \frac{\alpha}{\sqrt{\pi}} \frac{x_0 \exp(-x_0^2)}{\Psi(x_0)} \right] \pm 2x_0 \sqrt{\alpha \left(\nu_{E_i} + \nu_{E_e} \frac{T_e}{T_i} \right) \tau}, \quad (91)$$

where

$$\nu_{E_e} = \frac{8\pi Z^2 e^4 n \ln \Lambda}{A(2T_e)^{\frac{3}{2}}} \frac{\sqrt{m_e}}{m_p} \frac{\Psi(x_e)}{x_e} = \frac{3}{2} \sqrt{\pi} \frac{m_e}{m} \frac{Z^2}{Z_i} \nu_{B_e} \frac{\Psi(x_e)}{x_e} \quad (92)$$

and

$$\nu_{E_i} = \frac{8\pi Z^2 Z_i e^4 n \ln \Lambda_i}{A(2T_i)^{\frac{3}{2}}} \frac{\sqrt{m_i}}{m_p} \frac{\Psi(x_i)}{x_i} = 3 \sqrt{\frac{\pi}{2}} \frac{m_i}{m} \frac{Z^2}{Z_i^2} \nu_{B_i} \frac{\Psi(x_i)}{x_i}. \quad (93)$$

(iii). Energetic test ions ($u_{ith} \ll u \ll u_{eth}$) colliding with a field plasma consisting of electrons and a major ion species (i) as well as impurity species:

In this case, since $cx_0 = u/u_{eth} \ll 1$ and $x_0 = u/u_{ith} \gg 1$, ν_d reduces to

$$\nu_d = \frac{4\pi Z^2 \langle Z \rangle e^4 n \ln \Lambda}{A^2 m_p^2 u^3}, \quad (94)$$

where we have used Eq. (29) and $\langle Z \rangle$ as defined in Eq. (18).

To calculate the energy scattering operator we note that

$$\frac{x_e \exp(-x_e^2)}{\Psi(x_e)} \simeq \frac{3}{2} \sqrt{\pi}$$

and

$$\frac{\Psi(x_j)}{x_j} \simeq \frac{1}{2x_j^3}, \quad \exp(-x_j^2) \simeq 0 \quad (j = 1, 2, 3, \dots).$$

Thus

$$x_n^2 = x_0^2 - 2\nu_{E_e} \tau \left[x_0^2 - \frac{3}{2} \alpha \frac{T_e}{T_i} \right] - 2\nu_{E_i} \tau x_0^2 \pm 2x_0 \sqrt{\alpha \left(\nu_{E_i} + \nu_{E_i} \frac{T_e}{T_i} \right) \tau} \quad (95)$$

where

$$\nu_{E_e} \simeq \frac{8\pi Z^2 e^4 n \ln \Lambda}{A(2T_e)^{\frac{3}{2}}} \frac{\sqrt{m_e}}{m_p} \frac{2}{3\sqrt{\pi}} = \frac{m_e}{m} \frac{Z^2}{Z_i} \nu_{B_e} \quad (96)$$

and

$$\nu_{E_i} \simeq \frac{8\pi Z^2 e^4 n \ln \Lambda}{A m_p^2 u^3} \sum_j \frac{Z_j^2 n_j \ln \Lambda_j}{2A_j n \ln \Lambda} = \frac{4\pi Z^2 [Z] e^4 n \ln \Lambda}{A m_p^2 u^3}, \quad (97)$$

where $[Z]$ has been defined in Eq. (17).

Eqs. (96) and (97) are accurate only when $x_e \ll 1$ and $x_i \gg 1$ respectively. In energetic-ion scattering calculations, the former condition is very true. The latter condition is not always true, especially when the energetic particles relax to approach the energy of the thermal background plasma, in which case, it is better that we replace

$$\left(\frac{2T_i}{m_i} \right)^{3/2} / 2u^3 = \frac{1}{2x_i^3} \quad \text{by} \quad \frac{\Psi(x_i)}{x_i},$$

then Eq. (97) becomes

$$\nu_{E_i} \simeq \frac{8\pi Z^2 [Z] e^4 n \ln \Lambda}{A(2T_i)^{\frac{3}{2}}} \frac{m_i^{\frac{3}{2}}}{m_p^2} \frac{\Psi(x_i)}{x_i}. \quad (98)$$

3. Guiding center equations in different magnetic coordinate conventions

In practical Monte Carlo charged particle simulations, it is important to have a clear convention for the magnetic coordinates and the direction of the poloidal and toroidal currents, $g(\psi)$ and $I(\psi)$ respectively, as well as the sign of the rotational transform $\iota(\psi)$. The purpose of this section is to describe two commonly used magnetic coordinate conventions, then give their corresponding guiding center equations.

3.1 Representation of magnetic field in two coordinate conventions

The magnetic coordinate surfaces are defined by the toroidal magnetic flux ψ (ψ increases outwards from the magnetic axis), the poloidal angle θ and the toroidal angle ϕ . By means of these coordinate surfaces, we can define both the covariant basis vectors $\vec{\psi}$, $\vec{\theta}$, $\vec{\phi}$ and the contravariant basis vectors $\nabla\psi$, $\nabla\theta$, $\nabla\phi$. The two different coordinate conventions are constructed from each of the right-handed triplets (ψ, θ, ϕ) and (ψ, ϕ, θ) , as shown respectively in Fig. 1 and Fig. 2.

For both magnetic coordinate conventions, we define the rotational transform $\iota(\psi)$ as [6]:

$$\iota(\psi) \equiv \frac{d\psi_p}{d\psi} \equiv \frac{\nabla\psi_p}{\nabla\psi} \equiv \frac{1}{q(\psi)}, \quad (99)$$

where ψ_p is the poloidal magnetic flux, and $q(\psi)$ is the safety factor.

Naturally, here we should also have a convention for $\nabla\psi_p$, namely: the positive direction of the vector $\nabla\psi_p$ is in the same direction of $\nabla\psi$, — outwards from the magnetic axis — as indicated in Fig. 1 and 2. Under a selected magnetic coordinate convention, $\iota(\psi)$ reflects both the direction and magnitude of the rotational transform of the magnetic field lines.

For both magnetic coordinate conventions, we chose the same cylindrical coordinates (R, Φ, Z) as the reference in real space.

(i). The convention (ψ, θ, ϕ) :

The contravariant basis vectors $\nabla\psi$, $\nabla\theta$, $\nabla\phi$ form a right-handed system (Fig. 1). According to this convention The contravariant representation of the magnetic field \mathbf{B} is then

$$\mathbf{B} = \nabla\psi \times \nabla\theta + \nabla\phi \times \nabla\psi_p, \quad (100)$$

where $\nabla\psi \times \nabla\theta$ points in the $\vec{\phi}$ direction, and $\nabla\phi \times \nabla\psi_p$ points in the $\vec{\theta}$ direction. Thus $\vec{\phi}$ is the positive direction of the toroidal component of \mathbf{B} , and $\vec{\theta}$ is the positive direction of the poloidal component of \mathbf{B} .

The covariant representation of \mathbf{B} is written as

$$\mathbf{B} = g(\psi)\nabla\phi + I(\psi)\nabla\theta + \delta(\psi, \theta)\nabla\psi, \quad (101)$$

where we have the following important convention:

The positive direction of poloidal current $g(\psi)$ and toroidal current $I(\psi)$ are defined by the magnetic coordinate directions $\nabla\phi$ and $\nabla\theta$ according to the so called right-hand law. That is, if a positive poloidal current $g(\psi)$ flows in the $\nabla\theta$ direction, then it produces a positive toroidal component of \mathbf{B} (in the $\nabla\phi$ direction) according to right hand law. A positive toroidal current $I(\psi)$ should be in $\nabla\phi$ to produce a positive poloidal component of \mathbf{B} (in the $\nabla\theta$ direction).

In principle, it is possible to use other conventions to define the positive directions of the currents, for instance, we can suppose that the positive $g(\psi)$ is in $-\nabla\theta$ direction, then it leads to a different representation of the covariant \mathbf{B} .

(ii). The convention (ψ, ϕ, θ) :

The contravariant basis vectors $\nabla\psi, \nabla\phi, \nabla\theta$ form a right-handed system (Fig. 2). Under this convention, the contravariant representation of \mathbf{B} is now

$$\mathbf{B} = \nabla\theta \times \nabla\psi + \nabla\psi_p \times \nabla\phi, \quad (102)$$

where $\nabla\theta \times \nabla\psi$ is the toroidal component of \mathbf{B} , pointing in the direction of $\vec{\phi}$, and $\nabla\psi_p \times \nabla\phi$ is the poloidal component of \mathbf{B} , pointing in the direction of $\vec{\theta}$.

The covariant representation of \mathbf{B} is written as

$$\mathbf{B} = g(\psi)\nabla\phi + I(\psi)\nabla\theta + \delta(\psi, \theta)\nabla\psi. \quad (103)$$

According to this convention, to produce a positive toroidal B_ϕ ($\nabla\phi$ direction), the positive direction of $g(\psi)$ should be in the $-\nabla\theta$ direction. To produce a positive poloidal B_θ ($\nabla\theta$ direction), the positive direction of $I(\psi)$ should be in the $-\nabla\phi$ direction.

3.2 Guiding center equations for both conventions

(i). For the convention (ψ, θ, ϕ) :

This is the convention used in reference [5] to examine the ATF torsatron. From Eqs. (100), (101) and (99), the toroidal and poloidal canonical momenta are determined

$$p_\phi = e\rho_{\parallel}g - e\psi_p \quad (104)$$

and

$$p_\theta = e\rho_{\parallel}I + e\psi, \quad (105)$$

where p_ϕ and p_θ are the toroidal and poloidal canonical momenta of a charged particle, and the guiding center equations are

$$\dot{p}_\phi = -\left(\frac{e^2B}{m}\rho_{\parallel}^2 + \mu\right)\frac{\partial B}{\partial\phi}, \quad (106)$$

$$\dot{p}_\theta = -\left(\frac{e^2B}{m}\rho_{\parallel}^2 + \mu\right)\frac{\partial B}{\partial\theta}, \quad (107)$$

$$\dot{\phi} = -\left[\left(\frac{e^2B}{m}\rho_{\parallel}^2 + \mu\right)\frac{\partial B}{\partial\psi} + e\frac{\partial\Phi}{\partial\psi}\right]\frac{I}{\gamma} + \frac{e^2B^2}{m}\rho_{\parallel}\frac{1 + \rho_{\parallel}I'}{\gamma}, \quad (108)$$

$$\dot{\theta} = +\left[\left(\frac{e^2B}{m}\rho_{\parallel}^2 + \mu\right)\frac{\partial B}{\partial\psi} + e\frac{\partial\Phi}{\partial\psi}\right]\frac{g}{\gamma} + \frac{e^2B^2}{m}\rho_{\parallel}\frac{\tau - \rho_{\parallel}g'}{\gamma}, \quad (109)$$

$$\dot{\psi} = \left(\frac{e^2B}{m}\rho_{\parallel}^2 + \mu\right)\left(\frac{I}{\gamma}\frac{\partial B}{\partial\phi} - \frac{g}{\gamma}\frac{\partial B}{\partial\theta}\right) = -\frac{1}{\gamma}(\dot{p}_\phi I - \dot{p}_\theta g), \quad (110)$$

$$\dot{\rho}_{\parallel} = \frac{1}{\gamma}[(1 + \rho_{\parallel}I')\dot{p}_\phi + (\tau - \rho_{\parallel}g')\dot{p}_\theta], \quad (111)$$

where

$$\gamma = e[(1 + \rho_{\parallel}I')g + (\tau - \rho_{\parallel}g')I], \quad (112)$$

and $\Phi = \Phi(\psi)$ is the electric potential.

In this convention if we consider the case of a right-handed stellarator, the rotational transform of the magnetic field lines should be positive,

$$\tau(\psi) > 0,$$

so that the magnetic field lines trace in the direction of increasing (or decreasing) ϕ , i.e. $\nabla\phi$ (or $-\nabla\phi$) and increasing (or decreasing) θ , i.e. $\nabla\theta$ (or $-\nabla\theta$) (Fig. 1). Similarly, if we consider the case of a left-handed stellarator, the rotational transform should be negative.

The basic behaviour of a test particle orbit in both the magnetic coordinate space $(\nabla\psi, \nabla\theta, \nabla\phi)$ and the real space (R, Φ, Z) may be qualitatively predicted.

For a given right-handed stellarator ($\iota > 0$) with a positive poloidal current $g(\psi) > 0$ (in $\nabla\theta$ direction), a test ion with $\lambda = v_{||}/v = 1$, should travel in the direction of increasing $\nabla\phi$ (as $\lambda > 0$) and increasing $\nabla\theta$ (as $\iota(\psi) > 0$). The orbit follows a right-handed screw in the direction of $\nabla\phi$ in magnetic coordinate space.

In real space, the same test ion travels in the Φ direction (as $\lambda > 0$), whilst rotating clockwise. The orbit thus follows a right-handed screw in the Φ direction. The real orbit is completely determined by the right-handed magnetic field (which is determined by the magnetic field coil arrangement).

(ii). For the convention (ψ, ϕ, θ) :

This is the coordinate convention used at IPP Garching to describe W7AS. The corresponding guiding center equations are as follows:

From Eqs. (102), (103), and (99), the toroidal and poloidal canonical momenta are determined

$$p_\phi = e\rho_{||}g + e\psi_p, \quad (113)$$

$$p_\theta = e\rho_{||}I - e\psi, \quad (114)$$

and the guiding center equations are

$$\dot{p}_\phi = -\left(\frac{e^2B}{m}\rho_{||}^2 + \mu\right)\frac{\partial B}{\partial\phi}, \quad (115)$$

$$\dot{p}_\theta = -\left(\frac{e^2B}{m}\rho_{||}^2 + \mu\right)\frac{\partial B}{\partial\theta}, \quad (116)$$

$$\dot{\phi} = +\left[\left(\frac{e^2B}{m}\rho_{||}^2 + \mu\right)\frac{\partial B}{\partial\psi} + e\frac{\partial\Phi}{\partial\psi}\right]\frac{I}{\gamma} + \frac{e^2B^2}{m}\rho_{||}\frac{1 - \rho_{||}I'}{\gamma}, \quad (117)$$

$$\dot{\theta} = -\left[\left(\frac{e^2B}{m}\rho_{||}^2 + \mu\right)\frac{\partial B}{\partial\psi} + e\frac{\partial\Phi}{\partial\psi}\right]\frac{g}{\gamma} + \frac{e^2B^2}{m}\rho_{||}\frac{\iota + \rho_{||}g'}{\gamma}, \quad (118)$$

$$\dot{\psi} = +\frac{1}{\gamma}(\dot{p}_\phi I - \dot{p}_\theta g), \quad (119)$$

$$\dot{\rho}_{||} = \frac{1}{\gamma}[(1 - \rho_{||}I')\dot{p}_\phi + (\iota + \rho_{||}g')\dot{p}_\theta], \quad (120)$$

where

$$\gamma = e[(1 - \rho_{||}I')g + (\iota + \rho_{||}g')I]. \quad (121)$$

In this convention if we consider the case of a left-handed stellarator, the rotational transform of the magnetic field lines should be positive,

$$\iota(\psi) > 0,$$

so that the magnetic field lines trace in the direction of increasing (or decreasing) ϕ , i.e. $\nabla\phi$ (or $-\nabla\phi$) and increasing (or decreasing) θ , i.e. $\nabla\theta$ (or $-\nabla\theta$) (Fig. 2). Similarly,

if we consider the case of a right-handed stellarator, the rotational transform should be negative.

The basic behaviour of the particle orbit may be predicted under this coordinate convention:

For a given left-handed stellarator ($\iota > 0$) with a positive poloidal current $g(\psi) > 0$ (in $-\nabla\theta$ direction), a test ion with $\lambda = v_{\parallel}/v = 1$, should travel in the direction of increasing $\nabla\phi$ (as $\lambda > 0$) and increasing $\nabla\theta$ (as $\iota(\psi) > 0$). The orbit follows a left-handed screw in the direction of $\nabla\phi$ in magnetic coordinate space.

In real space, the same test particle should have a left-handed rotational orbit going in the direction of Φ . It is determined only by the configuration of the magnetic field in real space and is independent of the conventions of the magnetic coordinate systems.

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Figure captions

Fig. 1. A sketch of magnetic coordinate convention (ψ, θ, ϕ).

Fig. 2. A sketch of magnetic coordinate convention (ψ, ϕ, θ).

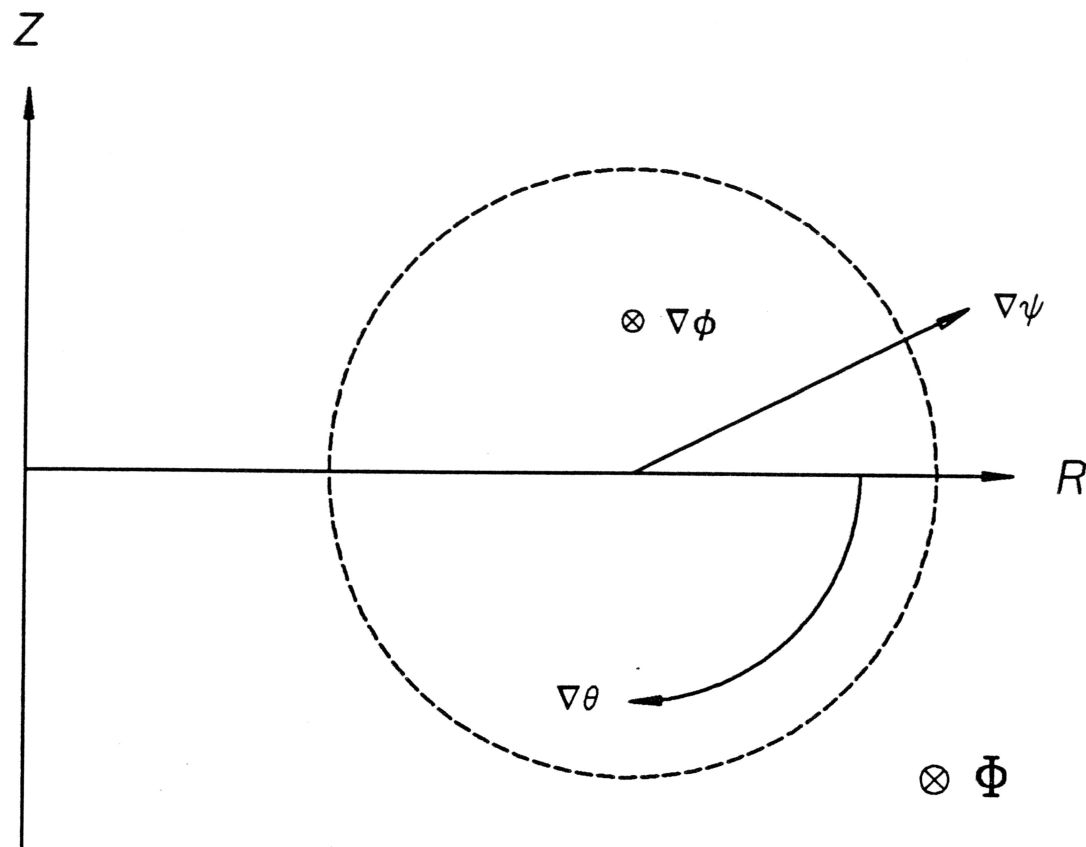


Fig. 1

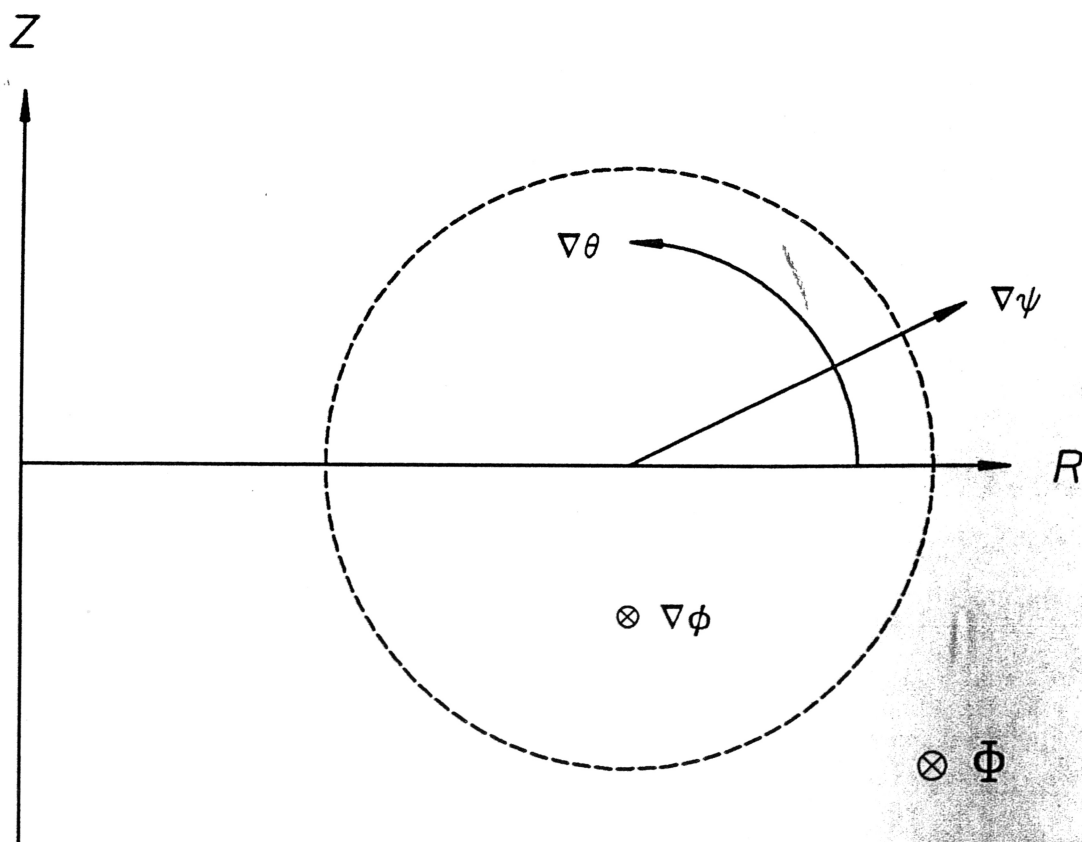


Fig. 2