Abstract. The absorption of radio-frequency waves in the ion-cyclotron range of frequencies (ICRF) in fusion plasmas is adequately described in the frame of the quasilinear theory. A peculiarity of ICRF heating is to increase the fraction of trapped particles, whose guiding-center trajectories are typically banana orbits with finite width. One possible way to properly account for the effects due to the finite-width orbits is provided by the orbit-averaged quasilinear theory. Here, we propose a routine for the evaluation of the orbit-averaged quasilinear diffusion tensor, given the the wave fields from the full wave code TORIC. Particular care is taken in the evaluation of the contribution of each wave-particle resonance as well as for the transition between the two regimes of correlated and uncorrelated resonances along the orbit. We discuss the quasilinear diffusion coefficient thus obtained and validate the result by comparing the power deposition profile computed from the orbit-averaged quasilinear operator with the one determined by TORIC. For future applications, a novel algorithm for the calculation of the corresponding Monte Carlo operators is also presented.

1. Introduction
The evolution of the ion distribution function in the presence of high frequency waves in the ion-cyclotron (IC) range of frequencies is usually described in the frame of the quasilinear (QL) theory [1, 2, 3, 4, 5]. A common approximation is to surface average the quasilinear operator, which is equivalent to assuming that all the resonant particles are tied to magnetic field lines. This is a good approximation for the description of waves interacting with the thermal bulk of particles. However, IC fast-wave heating typically increases the fraction of energetic deeply trapped ions characterized by large banana orbits. To describe properly the finite banana-width effects it is necessary to follow the particles along their guiding-center drift orbits [6]. The Doppler shift in the wave-particle resonance condition, moreover, is usually calculated by retaining in the wave fields description only one toroidal wavenumber (typically the dominant value of the antenna spectrum), and neglecting the contribution of the poloidal wavenumber to the parallel component of the wave vector.

Here we relax these constraints: we present a routine which evaluates the resonance kernel of the quasilinear operator by following the guiding-center orbits, and takes into account all Fourier components of the wave field calculated with the full-wave code TORIC [7]. For each Fourier component, the Doppler shift is evaluated at the resonant position corresponding to its poloidal and toroidal wave numbers and the local particle velocity.
The orbit-averaged quasilinear theory upon which our calculations are based is briefly reviewed in section 2. The algorithm and the first numerical results are then reported in section 3. In particular, the quasilinear diffusion coefficient is studied in relation to the different topologies of ion orbits. As a check, we have compared the heating rate predicted by the QL operator assuming a Maxwellian distribution function, with the power deposition profile evaluated by TORIC under the same assumption. In section 4 we present a novel algorithm to compute numerically the Monte Carlo operators in a general set of invariants starting from the orbit-averaged quasilinear operator. In the last section we draw preliminary conclusions.

2. The orbit-averaged quasilinear diffusion tensor

In axisymmetric tokamak plasmas, the unperturbed ion orbits are characterized by three adiabatic invariants [1, 8], i.e., the energy \( \varepsilon \), the magnetic moment \( \mu \) and the toroidal momentum \( P_\varphi \), together with the poloidal and toroidal angles \((\vartheta, \varphi)\) of the ion guiding center and the phase \( \phi_v \) of the fast ion gyration around the guiding center. Along with \( \vec{I} = (\varepsilon, \mu, P_\varphi) \), it is useful to consider also arbitrary (curvilinear) coordinates \( \vec{I} = (I^1, I^2, I^3) \) in the space of invariants; the value of \( \vec{I} \) determines the guiding-center trajectory which evolves either with (trapped particle) or without (passing particle) change of the sign of the velocity component parallel to the local confining magnetic field. In both cases, the motion in \( \vec{I} \) is periodic, and the corresponding time period is referred to as the bounce time \( \tau_b \), which depends on the particle invariants \( \vec{I} \). On a slower time scale the evolution of the particle distribution function \( F \) of a given ion species is governed by the balance between resonant wave-particle interactions and collisions. In the quasilinear picture, the kinetic equation describing this evolution is [1, 3, 4]

\[
\frac{\partial F}{\partial t} = Q_{\text{avg}}(F) + C_{\text{avg}}(F) \quad \text{with:} \quad Q_{\text{avg}}(F) = \frac{1}{\sqrt{|g|}} \frac{\partial}{\partial I^\alpha} \left( \sqrt{|g|} D_{\alpha\beta} \frac{\partial F}{\partial I^\beta} \right)
\]

(1)

where \( F = F(\vec{I}) \), \( D_{\alpha\beta} \) is the orbit-averaged quasilinear diffusion tensor, and \( C_{\text{avg}}(F) \) is the orbit-averaged collision operator.

The QL operator in (1) is in divergence form with \( g \) being the metric tensor associated with the generic set of invariants \( \vec{I} \). For example, on making use of the action variables \( I^\alpha = J^\alpha \), one finds that the metric is Euclidean and, thus, \( |g| = 1 \), while, in the case of \( \vec{I} = (\varepsilon, \mu, P_\varphi) \), one can show \( |g| \propto \tau_b^2 \) [3]. The QL diffusion tensor can be written as

\[
D_{\alpha\beta} (\vec{I}) = \frac{1}{2} \text{Re} \left\{ \frac{1}{\tau_b} \int_0^{\tau_b} dt \int_0^{2\pi} \frac{d\phi_v}{2\pi} \Delta^\alpha(t, \phi_v)^* \int_t^\infty dt' \Delta^\beta(t', \phi_v) \right\}.
\]

(2)

The first integral is the average over the bounce period, the second integral comes from the gyro-average over the fast phase \( \phi_v \), and the third integral is the result of integrating the linearized Vlasov equation along the unperturbed particle orbits. As a consequence of axisymmetry [3, 4], the averages in (2) can be shown to be equivalent to the standard orbit average of reference [1]. The quantities \( \Delta^\alpha \) are evaluated on the particle trajectory corresponding to invariants \( \vec{I} \), with \( m\vec{a} = Ze(E + \vec{v} \times \vec{B})/c \) being the Lorentz force due to the radio-frequency fields. In our study, the wave fields are provided by the full-wave code TORIC [7] which makes use of the spectral representation \( \vec{E} = \sum_{(m,n)} \vec{E}_{m,n}(\psi), \vec{B}_{m,n}(\psi) e^{i(m\vartheta+n\varphi)} - i\omega t, \psi \) being a label of the magnetic surfaces. Due to the contravariant nature of the QL diffusion tensor, \( D_{\alpha\beta} \) of (2) can be readily transformed into any other coordinate system.

Following the classical derivation [2], we obtain, for a single cyclotron harmonic \( p \) and neglecting the parallel component of the electric field,

\[
D_{\alpha\beta} = \frac{Ze^2}{2m^2} \text{Re} \left\{ \sum_{\nu_1, \nu_2} \frac{1}{\tau_b} \int_0^{\tau_b} dt \Pi_{\nu_1}(t)^* e^{-i\chi_{\nu_1}(t)} \int_0^{+\infty} dt' \Pi_{\nu_2}(t-t') e^{i\chi_{\nu_2}(t-t')} \right\},
\]

(3)
where, for brevity, \( \nu = (m, n) \), and

\[
\Pi^\alpha_\nu(t) = \frac{v_\perp}{\sqrt{2}} \left[ J_{p-1}(k_\perp \rho) E^+_\nu e^{-i\delta} + J_{p+1}(k_\perp \rho) E^-_\nu e^{i\delta} \right] X^\alpha, \\
\chi_\nu(t) = \int_0^t (p\Omega_\nu - \omega + k_\parallel v_\parallel) dt'.
\]  

Here, \( \Omega_\nu \) is the ion cyclotron frequency, \( J_p \) are Bessel functions, \( E^\pm_{\nu} \) are the rotating components of the wave electric field, \( \delta \) is a phase shift, and \( \vec{X} = (X^\alpha) \) is a vector field over the space of invariants. In equations (4) \( v_\parallel \) and \( v_\perp \) are to be expressed in terms of the invariants (hereafter, \( \parallel \) and \( \perp \) are defined with respect to the direction of the local magnetic field), \( k_\parallel \) is obtained from \( m, n \), and \( k_\perp \) is then computed from the cold-plasma dispersion relation for the fast root. It is worth noting that the phase \( \chi_\nu(t) \) is the integral of a periodic function (since the guiding center motion is periodic in \( \vartheta \)), but is not periodic itself. The integrals in (3) are evaluated using the stationary phase method, the stationary-phase points being defined by the usual Doppler-shifted resonance condition \( p\Omega_\nu - \omega + k_\parallel v_\parallel = 0 \). Hereafter we denote \( t_{\nu,j} \) the transit time of the guiding center at the resonance positions labelled by the index \( j = 1, 2, \ldots \). It is implicitly assumed that collisions decorrelate the wave-particle phase over times longer than a bounce period, thereby effectively suppressing resonances with harmonics of the bounce frequency [9]. On applying the stationary phase method, particular care must be taken for those stationary-phase points that hit the boundary of the integration domain. Finally we obtain a relatively simple approximation of (3),

\[
\tilde{D}_{\text{rt}}^{\alpha\beta} \approx \frac{Z^2 e^2}{2m^2} \frac{1}{\tau_b} \Re \left\{ \sum_{\nu_1} \left( \sum_{j_{\nu_1}} T^\alpha_{\nu_1,j_{\nu_1}} \right) \times \sum_{\nu_2} \left( \sum_{j_{\nu_2}} T^\beta_{\nu_2,j_{\nu_2}} \right) \right\},
\]

where for each \( \nu \) the index \( j_\nu \) runs over all resonances within one period. As well known [2, 10], when resonances are well separated in the sense of the stationary phase evaluation, there are two of them for passing ions, and four for trapped ions. In this case each contribution is given by the non-degenerate stationary-phase formula

\[
T^\alpha_{\nu,j} = \Pi^\alpha_0(t_{\nu,j}) \mathcal{W}_\nu(t_{\nu,j}) = \Pi^\alpha_0(t_{\nu,j}) \left| \frac{2\pi}{\chi^{(2)}_\nu(t_{\nu,j})} \right|^2 e^{\frac{i}{2} \text{sgn}(\chi^{(2)}_\nu(t_{\nu,j}))} \chi_\nu(t_{\nu,j}).
\]

where \( \chi^{(n)}_\nu = d^n \chi_\nu / dt^n \). Resonances can merge in pairs, however, for particles either on banana orbits with reflection point close to resonance, or on passing orbits nearly tangential to the cyclotron layer. In such cases the second-order derivative of the phase at resonance is small and the denominator in (6) blows up; for a correct evaluation the phase correlation between the two resonances cannot be neglected and their combined contributions take the form [2]

\[
T^\alpha_{\nu,j} = \Pi^\alpha_0(\Theta_j) \mathcal{W}_\nu(\Theta_j) = \Pi^\alpha_0(\Theta_j) 2\pi e^{i\chi_\nu(\Theta_j)} [\chi^{(2)}_\nu(\Theta_j)]^{-\frac{1}{2}} \text{Ai}(\chi^{(1)}_\nu(\Theta_j)[\chi^{(3)}_\nu(\Theta_j)]^{-\frac{1}{2}}),
\]

where \( \text{Ai} \) is the Airy function, and the argument \( \Theta_j \) is defined as the point between the two considered resonances where the second derivative vanishes, \( \chi^{(2)}_\nu(\Theta_j) = 0 \). We have investigated numerically the transition between the case of two isolated and two merging resonances (cf. section 3), and adopted a matching procedure similar, but not identical, to that proposed in [10].

For sake of simplicity, in this paper we limit our analysis to the dominant [Appendix B of [2]] diagonal terms in the double sum (5) (the significance of the off-diagonal terms will be addressed
in the future). On making use of (6) and (7), the quasilinear diffusion tensor takes the form

\[ \bar{D}_{\alpha\beta} \approx \sum_{\nu} \sum_{j_{\nu}} D_{\nu,j_{\nu}} X_{\nu,j_{\nu}}^\alpha X_{\nu,j_{\nu}}^\beta, \] (8)

where \( D_{\nu,j} \) are positive coefficients and \( \vec{X} = (X_{\nu,j}^\alpha) \) is the vector field \( \vec{X} = (X^\alpha) \) evaluated at either \( t_{\nu,j} \) for well-separated resonances or \( \Theta_{j} \) for merging resonances. The quasilinear diffusion tensor thus obtained (8) amounts to a sum of dyadics with positive coefficients, hence it is symmetric and positive definite [3].

The dyadic structure of \( \bar{D}_{\alpha\beta} \) is crucial for the calculation of the Monte Carlo, cf. section 4. Let us recall that in a Monte Carlo (MC) code the invariants of a given particle are periodically updated according to

\[ I^\alpha \mapsto I^\alpha + \Delta I^\alpha, \]

\[ \Delta I^\alpha = \ddot{I}^\alpha \Delta t + \sqrt{2\Delta t} \sum_{a=1}^{3} A^\alpha_a \xi_a, \] (9)

where \( \xi_a \) are random numbers sampled from a normal distribution of zero mean and unit variance; the time-derivatives \( \ddot{I}^\alpha \) of the expectation values and the vectors \( \vec{A}_a = (A^\alpha_a) \) should be evaluated from \( \bar{D}_{\alpha\beta} \) according to [4]

\[ \ddot{I}^\alpha = \frac{1}{\sqrt{|g|}} \frac{\partial}{\partial I^\beta} \left( \sqrt{|g|} \bar{D}_{\alpha\beta} \right), \quad \bar{D}_{\alpha\beta} = \sum_{a=1}^{3} A^\alpha_a A^\beta_a. \] (10)

By inspection of the second equation in (10) one can see that the coefficients \( A^\alpha_a \), regarded as a matrix, amount to the square root of \( \bar{D}_{\alpha\beta} \). The analytical calculation of the derivative of the expectation value, on the other hand, can be rather cumbersome [4]. In section 4 we propose a new algorithm for the calculation of the Monte Carlo operators (10).

3. Algorithm implementation and numerical results
In this section, the algorithm for the evaluation of the quasilinear diffusion tensor (8) is briefly outlined. Then, we report about the first numerical results that provide a rather detailed study of the quasi-linear diffusion tensor and its relationship to the topology of guiding-center trajectories, together with an estimate of the heating rate.

3.1. Numerical evaluation of the quasilinear diffusion tensor from TORIC wave fields
The value of the quasilinear diffusion tensor (8) depends on the Fourier coefficients of the wave electric field, and on the specific guiding-center trajectory corresponding to the set of invariants \( \vec{I} \).

The numerical evaluation of the diffusion tensor is obtained by integrating the guiding-center drift equations [6] by means of an ad hoc routine based upon the explicit solver LSODE [12], then locating the resonances along the trajectory and evaluating their contributions to the sum (8). The guiding-center trajectories have been sampled according to a uniform mesh in energy \( \varepsilon \) and an adapted non-uniform mesh in the normalized magnetic moment \( \Lambda = \mu B_{eq}/\varepsilon \), where \( B_{eq} \) is the value of the magnetic field at the point of the external equatorial transit of the particle; instead of \( P_{\psi} \), we use the radial position \( \psi_{eq} \) of the equatorial transit, uniformly discretized, together with the sign \( \sigma_\parallel \) of the the parallel velocity. For each point \( (\varepsilon, \Lambda, \psi_{eq}, \sigma_\parallel) \) of the grid the value of \( \bar{D}_{\alpha\beta} \) is computed and written onto a table, which can subsequently be read and interpolated by any Monte Carlo code. The frames (a) and (b) of figure 1 show an example of poloidal projections of the guiding-center trajectory of passing and trapped particles respectively. The bullets mark the
Figure 1. Poloidal projections of the guiding-center trajectory of passing (a) and trapped (b) particles. The bullets mark the wave-particle resonance positions for $m = -15$ (green), $m = 0$ (magenta), $m = +15$ (light blue) and the same $n = +12$. The vertical dashed line is the resonance position of the $(m = 0, n = 0)$ mode, i.e. without Doppler shift.

Figure 2. The Resonance kernel $W_\nu = \sum_j |W_{\nu,j}|^2$ for passing (a) and trapped (b) particles as function of $x = \omega / (\Omega_c + k_\parallel v_\parallel)$. By varying $x$ the resonance layer moves from the high field side to the low field side of the guiding-center trajectories.

wave-particle resonance positions for the different values of $m$, all the resonances calculated for the same $n = +12$. As reference, the vertical dashed line corresponds to the cyclotron resonance in the absence of Doppler shift. For passing particles (frame (a)) the resonances with the same $(m, n)$ values are almost vertically aligned. This is not the case for trapped particles (frame (b)) where the Doppler shift is influenced by the strong variations of $v_\parallel$ along the guiding-center trajectory. In particular, $v_\parallel$ changes sign when passing over the banana tips: for this reason the resonances in the internal and external part of the trajectory are Doppler-shifted in opposite directions.
Figure 3. Diffusion coefficient $\bar{D}^{\varepsilon\varepsilon}$ as function of $\Lambda$ for $\psi_{\text{eq}} = 0.5$ and $\sigma_v = +1$.

As an example of the transition from isolated resonances (6) to the phase-correlated regime (7), figure 2 shows the sum of the resonance kernels $W_\nu = \sum_j |W_{\nu,j}|^2$ with $\nu = (m = 10, n = 12)$ for passing and trapped particles, respectively frame (a) and (b). The quantity $W_\nu$ is plotted as function of $x = \omega/(\Omega_c + k_{||} v_{||})$; with increasing $x$ the resonances move from the high (left) to the low (right) field side of the guiding-center trajectory. In the case of figure (2.a), for $0.8 < x < 0.84$ the resonances are phase-correlated and the resonance kernel is described by the Airy function, cf. (7). In the interval $0.84 < x < 0.98$ the resonances are well separated and the stationary phase formula (6) is applied. For $x > 0.98$ the resonances are phase-correlated again.

In the case of trapped particles, figure (2.b), the picture is more complicated. The first peak on the left originates from the contribution of two pairs of correlated resonances; this happens when the resonance layer is approximately close to the banana tips. Then, a first plateau corresponding to four uncorrelated resonances develops into a second smaller peak which is due to a pair of correlated resonances together with two uncorrelated; this happens when the resonance layer, moving towards the low field side, leaves the inner branch of the banana orbit. At last, after a second plateau, where only two uncorrelated contributions are significant, a third peak appears when the two remaining resonances becomes correlated. The transition between the two regimes described by equations (6) and (7) is implemented by imposing a threshold on the value of the argument of the Airy function in equation (6); the specific value has been selected in order to ensure the continuity of the resonance kernel.

Figure 3 shows $\bar{D}^{\varepsilon\varepsilon}$ as function of the normalized magnetic moment for different values of energy and $\psi_{\text{eq}} = 0.5$, $\sigma_v = +1$, $n_{\varphi} = +12$ and summing over $m$ in the range $-15 \leq m \leq +15$. The transition from passing to trapped particles is visible as a sharp feature of $\bar{D}^{\varepsilon\varepsilon}$ pattern around $\Lambda = \Lambda_c = B_{\text{eq}}/B_{\text{max}} \approx 0.8$. The $\bar{D}^{\varepsilon\varepsilon}$ peak is in correspondence of trapped particles which are in resonance with the wave close to their banana tips. If $\Lambda$ is increased further, the particle is reflected before encountering the resonance and $\bar{D}^{\varepsilon\varepsilon}$ rapidly decreases to zero.

3.2. An estimate of the heating rate
As an order-of-magnitude validation we compare the power deposition profiles predicted by TORIC and the heating rate profile predicted by the quasilinear operator evaluated above. Without solving the kinetic equation (1), in both cases we assume that the distribution function $F(\vec{I})$ is a Maxwellian $F_M(\varepsilon)$. If we use as set of invariants $\vec{I} = (\varepsilon, \Lambda, \bar{\psi})$, with $\bar{\psi}$ the third
where $F_p(\psi) = d\Psi_p/d\psi$, with $\Psi_p$ the poloidal flux, $V(\psi)$ is the specific volume of the magnetic surface $\psi$, and $\bar{D}^{\epsilon\epsilon}_{rf}$ is calculated according to (8). In order to be consistent with the model of TORIC, in equation (11) we consider the limit of well passing particles $\bar{\psi} \approx \psi$. Figure (4) shows the radial power deposition profiles: the red line has been obtained implementing equation (11) given the diffusion coefficients computed in section 3.1, whereas the blue line is obtained from TORIC. The profile predicted by QL coefficient is broader than the profile computed by TORIC. This difference can be explained by the finite orbit widths, which are not included in TORIC model. However, this broadening can also be due to the neglected off-diagonal terms in (5). This will be investigated in the future. Moreover, the two profiles in Figure (4) exhibit a different behavior near the magnetic axis. However, the power balance is not affected by this discrepancy since upon integrating over $\psi$ the power density is weighted with a specific volume which is small for $\psi \to 0$. In fact, the total absorbed power computed from the two deposition profiles are in good agreement, the values being: 0.667 MW from TORIC and 0.704 MW from integrating equation (11) over $\psi$, both for 1 MW of absorbed ICRF power.

4. Numerical evaluation of Monte Carlo operators

In the evaluation of the Monte Carlo (MC) operator (10), one must perform the derivatives of the quasilinear diffusion tensor. To avoid to perform these derivatives analytically, we propose to calculate numerically $\dot{I}^\alpha$ by using the divergence of the quasilinear diffusion tensor $\bar{D}^0_{\alpha\beta}$ written in the form

$$
\dot{I}^\alpha = \sum_\nu \sum_{j_\nu} \left\{ X^\alpha_{\nu,j_\nu} L_{X^\alpha_{\nu,j_\nu}} D_{\nu,j_\nu} + D_{\nu,j_\nu} [ L_{X^\nu_{\nu,j_\nu}} X^\alpha_{\nu,j_\nu} + X^0_{\nu,j_\nu} \text{div} \bar{X}_{\nu,j_\nu} \} \right\},
$$

where $L_{X^\nu_{\nu,j_\nu}} = X^\alpha_{\nu,j_\nu}(\partial/\partial I^\alpha)$. The terms in equation (12) amount to the derivative of scalar functions, i.e. $D_{\nu,j_\nu}$ and $X^0_{\nu,j_\nu}$, along the integral lines of the vector field $\bar{X}_{\nu,j_\nu}$ together with $\text{div} \bar{X}_{\nu,j_\nu}$. The latter can also be related to $L_{X^\nu_{\nu,j_\nu}}$ in virtue of the identity

$$
L_{X^\nu_{\nu,j_\nu}} (dV_I) = (\text{div} \bar{X}_{\nu,j_\nu}) dV_I.
$$
where \(dV_I = \sqrt{|g|} dI\) is the volume form in the space of invariants. The volume element \(dV_I\) is approximated by the volume enclosed by the four points of a three-dimensional simplex (convex hull of the simplex) with small-enough edges. On the other hand, the derivative \(L_{\vec{X}_{\nu,j\nu}}\) applied to a generic function is approximated by symmetric finite differences upon moving upward and backward along the integral lines of \(\vec{X}_{\nu,j\nu}\) with an explicit forth-order Runge-Kutta scheme. In doing this, the properties of the simplex enclosing a convex region significantly simplifies the calculation of the volume \(dV_I\) at the new positions. At last, the vectors \(\vec{A}_\alpha\) are computed by taking the square root of \(\bar{D}^{\alpha\beta}_{\nu\nu}\) regarded as a matrix.

5. Conclusions

We have presented the algorithms and numerical implementation for the evaluation of the orbit-averaged quasilinear operator in the ion cyclotron range of frequencies. Starting from the wave fields calculated by a full-wave solver, such as TORIC, and following the guiding-center orbits we have computed the coefficients of the quasilinear diffusion operator in a general axisymmetric configuration. Particular attention has been devoted in calculating the resonance kernel of the wave-particle interaction. This has required to implement a numerical algorithm capable of dealing with all the possible kinds of guiding-center trajectories and relative positions of the resonance points. As a preliminary test, we have estimated the heating rate profile in the limit of Maxwellian distribution function, in order to compare it with the deposition profile calculated by TORIC. The agreement in the total heating rate is an important check, in view of the fact that no \textit{ad hoc} normalization of the wave fields have been made. The deposition profile calculated from the quasilinear diffusion coefficient is broader than that determined by TORIC: this difference can be explained by the finite orbit width, which are not included in TORIC model.

Finally, we have outlined the numerical algorithm necessary to derive the Monte Carlo operators in a general set of invariants starting from the orbit-averaged quasilinear coefficients evaluated in this work.

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