Implementing zero-banana-width quasilinear operator for fast ICRF simulations

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Abstract. Numerical simulations of plasma heating with waves in the ion cyclotron range of frequencies (ICRF) require to iteratively couple a solver for wave propagation in plasmas with a solver of the quasilinear kinetic equation. Among the codes developed for this purpose, the TORIC-SSFPQL package is characterized by its high execution speed. The kinetic code SSFPQL, however, was based on a somewhat simplified physical model, in which some important effects of the toroidal geometry were omitted. We have recently improved this model by taking into account in the zero–banana–width limit the influence of toroidal trapping on the ICRF quasilinear operator. To make the extended model compatible with the representation of the ion distribution functions as a truncated series of Legendre polynomials in the velocity pitch-angle adopted in SSFPQL, a special approach based on the multiprecision arithmetic had to be developed. We describe these new developments, and present first results obtained with the improved model.

1. Introduction

Plasma heating in the ion cyclotron range of frequencies (ICRF) has been extensively used in the past and present fusion devices, and should be available from the very beginning of the ITER operation [1]. This has motivated a considerable effort in simulating ICRF wave propagation and absorption. Since the wavelengths at these frequencies are comparable with the characteristic lengths of the plasma equilibrium profiles, asymptotic methods, such as geometrical optics, are not applicable, and the wave equations have to be solved numerically in full toroidal geometry, implying rather high execution costs. A brief review of the handful of full-wave codes developed and used for this purpose in the last few years is given by Budny and co-authors in [2].

During ICRF heating the distribution functions of the resonant species deviate appreciably from Maxwellians because of the production of important populations of energetic ions. In turn, suprathermal ions influence the propagation and absorption of the waves. As a consequence, a fully consistent simulation of ICRF heating requires the simultaneous solution of the full–wave

equations and of the quasilinear kinetic equation for the heated ion species [3–6], thereby further increasing the computational costs. The kinetic code is also needed to predict the collisional redistribution of the absorbed high-frequency (hf) power among different species.

The numerical complexity of the problem can be considerably reduced by omitting in the kinetic equation some details of the physics which are important to determine the fate of the most energetic ions produced by resonant ion-cyclotron (IC) interactions, but have only little influence on wave propagation and absorption. The kinetic code `SSFPQL` [7] which has been coupled to the full-wave code `TORIC` [8] looks for the steady-state solution of the surface-averaged kinetic equation, which amounts to neglect the final radial width of the guiding-center orbits of the heated ions. More importantly, in its first implementation the evaluation of the quasilinear (QL) diffusion coefficient was simplified by neglecting the effect of toroidicity on the parallel ion motion, thereby assuming that all ions cross IC resonances with constant velocity. In reality, the mirror force due to the inhomogeneity of the confining tokamak magnetic field has the consequence that some ions revert their parallel velocity near or even before reaching the resonance. The effect of toroidal trapping on wave absorption, although not dominant, is not really negligible.

In this note we discuss the control of round-off and truncation errors when solving the kinetic equation by expanding the solution in Legendre polynomials, and the extension of the numerical scheme used by the `SSFPQL` code in order to take into account toroidal trapping. In Section (2) we briefly recall the `SSFPQL` model and its implementation. In order to include the effects of toroidal trapping in the numerical scheme of this code it is necessary to avoid the accumulation of round-off errors in the numerical evaluation of certain recursive relations needed to build the QL diffusion coefficient in the Legendre representation. This has been achieved by using the multiprecision arithmetic facility offered by the `GMP` library [9]. In Section (3) the sources of truncation are discussed, and two empirical criteria to control them are proposed. In Section (4) we present the implementation of the effects of toroidal trapping in the numerical scheme of `SSFPQL`. An example of quasilinear distribution function in which these effects are taken into account is presented there. In the last Section we draw some conclusions and summarize what has yet to be done to complete this work.

2. The surface–averaged kinetic equation solved by `SSFPQL`

In the `TORIC-SSFPQL` package, the code `TORIC` solves the wave equation in axisymmetric toroidal plasmas [8], and the code `SSFPQL` evaluates the steady-state solution of the surface-averaged Fokker-Planck (FP) equation [7], written as balance between collisions, radio-frequency heating, and any other power source or sink S_j, including, if present, NBI heating [10]:

$$0 = \left(\frac{\partial F^{(i)}}{\partial t}\right)_{\rm coll} + \left(\frac{\partial F^{(i)}}{\partial t}\right)_{\rm rf} + S^{(i)} \ . \tag{1}$$

The linearized collisional operator describing test ions of species i colliding with a background Maxwellian plasma can be written as the sum of two differential operators acting separately on the speed v and on the pitch angle $\mu = v_\parallel/v$:

$$\left(\frac{\partial F^{(i)}}{\partial t}\right)_{\rm coll} = \mathcal{C}_v(F^{(i)}) + \mathcal{C}_\mu(F^{(i)}) \ .$$

The operator $\mathcal{C}_\mu(F^{(i)})$ describing pitch-angle scattering is proportional to the Legendre operator L_μ,

$$\mathcal{C}_\mu(F^{(i)}) = \frac{\Theta_c(v)}{2v^3}\, L_\mu(F^{(i)}) = \frac{\Theta_c(v)}{2v^3}\, \frac{\partial}{\partial \mu}\left[(1-\mu^2)\, \frac{\partial}{\partial \mu}\right] F^{(i)}(v,\mu) \ , \tag{2}$$

whose eigenfunctions are the Legendre polynomials $P_n(\mu)$. This peculiarity of the operator $\mathcal{C}_\mu$ suggests to represent the solution of Equation (1) as a superimposition of Legendre polynomials,

$$F^{(i)}(v,\mu;\psi) = \sum_{i=0} \tilde{F}_n^{(i)}(v;\psi)\ P_n(\mu)\ . \tag{3}$$

The two dimensional partial differential equation (1) is thereby reduced to a set of coupled ordinary-differential equations (ODEs) for the coefficients $\tilde{F}_n^{(i)}$ of the expansion.

The QL operator describing IC heating can be approximated as a purely perpendicular diffusion operator in velocity space,

$$\left(\frac{\partial F^{(i)}}{\partial t}\right)_{\rm rf} = \frac{1}{v_\perp}\frac{\partial}{\partial v_\perp}\left(v_\perp\ D_p(v_\perp)\ \frac{\partial F^{(i)}}{\partial v_\perp}\right)\ , \tag{4}$$

with the QL coefficient $D_p(v_\perp)$ for the pth harmonic heating given by

$$D_p(v_\perp) = D_0\ \left|J_{p-1}(\xi_\perp v_\perp) + \lambda_p\ J_{p+1}(\xi_\perp v_\perp)\right|^2\ . \tag{5}$$

Here $J_p(x)$ are the Bessel functions of the first kind, $v_\perp = v\sqrt{1-\mu^2}$, $\xi_\perp = k_\perp v_{\rm thi}/\Omega_{\rm ci}$, with $\Omega_{\rm ci} = Z_i eB/m_i c$ the cyclotron angular frequency, and $\lambda_p = (E_-/E_+)_{\rm res}$ is the wave polarization at the resonance, with E_- and E_+ the right and left circular components of the wave electric field. Transforming the QL operator to spherical coordinates and projecting on $P_n(\mu)$, the hf contribution to the equation for $\tilde{F}_n^{(i)}(v;\psi)$ becomes

$$\begin{aligned}\left(\frac{\partial \tilde{F}_n^{(i)}}{\partial t}\right)_{\rm rf} \quad = \quad \sum_m \frac{1}{v^2}\Bigg\{\frac{\partial}{\partial v}\left[v\ \left(\tilde{D}_p^{(0,0)}(n,m,v)\ v\,\frac{\partial}{\partial v} - \tilde{D}_p^{(0,1)}(n,m,v)\right)\right] \\ \left(\tilde{D}_p^{(1,0)}(n,m,v)\ v\,\frac{\partial}{\partial v} - \tilde{D}_p^{(1,1)}(n,m,v)\right)\Bigg\}\tilde{F}_m^{(i)}(v)\end{aligned} \tag{6}$$

with

$$\tilde{D}_p^{(j,k)}(n,m,v) = \int_{-1}^{+1}\left(\mu^j\frac{{\rm d}^j}{{\rm d}\mu^j}P_n\right)\ (1-\mu^2)\ D_p(v,\mu)\ \left(\mu^k\frac{{\rm d}^k}{{\rm d}\mu^k}P_m\right){\rm d}\mu \tag{7}$$

and $D_p(v,\mu) = D_p(\xi_\perp\, v\sqrt{1-\mu^2})$. The evaluations in closed form of the integrals (7) involving the Bessel functions (5) is made possible by using the multiplication theorem [11],

$$J_q(\xi_\perp\, v\sqrt{1-\mu^2}) = (1-\mu^2)^{q/2}\sum_{k=0}^{\infty}\frac{\mu^{2k}}{k!}\left(\frac{\xi_\perp v}{2}\right)^k\ J_{q+k}(\xi_\perp v)\,. \tag{8}$$

Using (8) in (7) we have

$$\begin{aligned}\tilde{D}_p^{(j,k)}(n,m,v) \quad = \quad D_0\ \sum_{s=0}^{\infty}\Bigg[\tilde{Q}_{p-1}^{(j,k)}(n,m,s)\mathcal{J}_{p-1,p-1}^s(\xi_\perp v) + 2{\rm Re}(\lambda_p)\ \tilde{Q}_p^{(j,k)}(n,m,s)\mathcal{J}_{p-1,p}^s(\xi_\perp v) + \\ |\lambda_p|^2\ \tilde{Q}_{p+1}^{(j,k)}(n,m,s)\mathcal{J}_{p,p}^s(\xi_\perp v)\Bigg]\,,\end{aligned} \tag{9}$$

where

$$\tilde{Q}_p^{(j,k)}(n,m,s) = \int_{-1}^{+1}\left(\mu^j\frac{{\rm d}^j}{{\rm d}\mu^j}P_n\right)\ (1-\mu^2)^{1+p}\ \mu^{2s}\ \left(\mu^k\frac{{\rm d}^k P_m}{{\rm d}\mu^k}\right){\rm d}\mu \tag{10}$$

and

$$\mathcal{J}^s_{p,q}(\xi_\perp v) = \left(\frac{\xi_\perp v}{2}\right)^s \sum_{r=0}^{s} \frac{1}{r!\,(s-r)!} J_{p+r}(\xi_\perp v)\; J_{q+s-r}(\xi_\perp v)\,. \tag{11}$$

Once the coefficients of the kinetic equations are calculated the set of ODEs in the variable v are solved with cubic–Hermite finite-element technique, the same used in `TORIC` code.

The critical numerical issue here is the evaluation of the integrals $\tilde{Q}_p^{(j,k)}(n,m,s)$. More precisely, we have to calculate the following three sets of integrals

$$X_p(n,m,k) = \int_{-1}^{+1} P_n(\mu)\;(1-\mu^2)^{1+p}\;\mu^k\;P_m(\mu)\mathrm{d}\mu \tag{12}$$

$$Y_p(n,m,k) = \int_{-1}^{+1} P_n(\mu)\;(1-\mu^2)^{1+p}\;\mu^k\;\left(\mu\frac{\partial P_m}{\partial \mu}\right)\mathrm{d}\mu \tag{13}$$

$$Z_p(n,m,k) = \int_{-1}^{+1} \left(\mu\frac{\partial P_n}{\partial \mu}\right)\;(1-\mu^2)^{1+p}\;\mu^k\;\left(\mu\frac{\partial P_m}{\partial \mu}\right)\mathrm{d}\mu \tag{14}$$

Since Legendre polynomials are characterized by oscillations, whose period decreases when approaching the domain boundaries ± 1 and with increasing order of the polynomial, it is unfeasible to evaluate these integrals numerically with sufficient accuracy. They satisfy, however, a set of two-dimensional, two-way recurrence relations. Unfortunately these relations are not stable against round-off error in the forward direction [12]. While totally negligible for Legendre polynomials up to a certain order, the round-off errors rapidly spoil any further evaluation when this order is exceeded. Working in IEEE 64-bit floating-point arithmetic typical of double-precision Fortran implementations, the maximum order of the polynomials which can be included is thereby limited to between 20 and 25. While this number might seem rather large, it turns out to be insufficient to guarantee convergence of the solution to a positive definite distribution function in a sufficiently large energy domain as soon as the QL operator is dominant over the collisional one. Empirically, this occurs when the local power deposited in the ions by IC resonances exceeds a fraction of Watt/cm^3, the precise limit depending on the collisionality of the plasma. The limitation is even more severe, if the simultaneous presence of NBI drives the distribution functions further away from Maxwellians already in an intermediate range of energies.

An important property of the recurrence relations (12,13,14) is that only rational numbers are involved both in the coefficients of the relation themselves and in the starting values [4]. Therefore, the use of the arithmetic of rational numbers offers a convenient way of circumventing the round-off error problem: the recurrence relations are evaluated using the rational representation of the numbers, and only one final division is needed to convert the result to a floating-point number. This makes the round-off errors equal to machine precision. One faces the problem, however, that the recurrence relations involve fractions of very quickly increasingly large integers, which cannot be represented with the integer arithmetic of standard compilers. This obstacle is removed by using the long–integer arithmetic of the multi-precision `GMP` library [9]. A first implementation of long–integer arithmetic for this purpose was made using `Mathematica` [13]. This, however, implied preparing a very large table of data to be read in the initialization phase of `SSFPQL`; the order of the Legendre expansion, moreover, cannot exceed the order available in this table. In addition, for tables extending to polynomials of order sixty or more, it is appreciably faster to calculate the integrals with the `GMP` library rather than to read them from the external file created with `Mathematica`.

As an example, Figure (1) shows the execution time needed to evaluate $X_p(n,m,k)$ in the range $n,m \le N_L$, $k < 2(N_L+100)+3$, and $0 \le p \le 3$, varying the maximum order N_L of the Legendre polynomials included. Compared are the evaluation in Fortran using double and

quadruple floating-point precision, and with the `GMP` library. In all three cases the computational time increases quadratically with N_L, but the `GMP` library is almost an order of magnitude slower than Fortran in quadruple precision. Nevertheless, the increased overhead for `SSFPQL` is still very tiny, and is more than compensated by the gain in accuracy. In Figure (1) the results of the Fortran evaluation are plotted with dashed line when the accumulated error exceeds 100%. In practice, use of the `GMP` library is the only solution for $N_L > 20$.

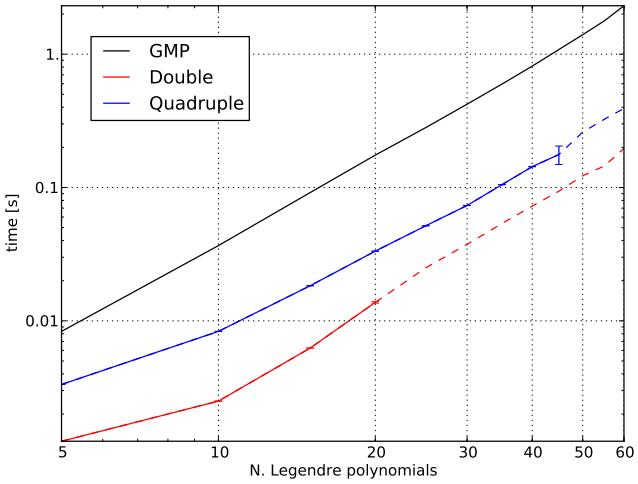

Figure 1. Computational time for double (`selected_real_kind(15, 307)`), quadruple (`selected_real_kind(33, 4931)`) floating-point arithmetic, and `GMP` multiprecision, required to calculate $X_p(n, m, k)$ as function of the maximum number of Legendre polynomials. Here $0 \leq p \leq 3$ and $0 \leq k \leq 2(N_L + 100) + 3$. The solid lines changes to dashed when the error becomes larger than 100%; in the `GMP` case the accuracy is always equal to the machine precision.

3. Controlling the truncation errors

In addition to the accumulation of round-off errors in the recurrence relations, the precision of `SSFPQL` solutions depends also on the errors introduced by truncating the sum (8) and, thus, the expansion of the QL diffusion coefficient in Bessel polynomials. In turn, the minimum number of polynomials which have to be included to ensure a good convergence of the Legendre representation of the QL operator determines how far the recursive relations discussed in the previous section have to be pushed.

While the r.h.s. of Equation (8) reduces to a single term for $\mu = 0$, convergence is slowest at the extrema $\mu = \pm 1$ of the velocity pitch-angle variable (ions with purely parallel velocity). In particular, at these points the slowest convergence of the series is when $q = 0$, where (8) becomes

$$\sum_{k=0}^{K=\infty} \frac{1}{k!} \left(\frac{x}{2}\right)^k J_k(x) = 1\,. \tag{15}$$

The requirement that (15) is satisfied within a given numerical accuracy selects the minimum number of terms to be retained in the numerical evaluation of the series (8). Figure (2.left) shows the difference between the truncated l.h.s. of (8) (evaluated in double precision) and unity as function of the argument x of the Bessel functions, and the number K of the terms

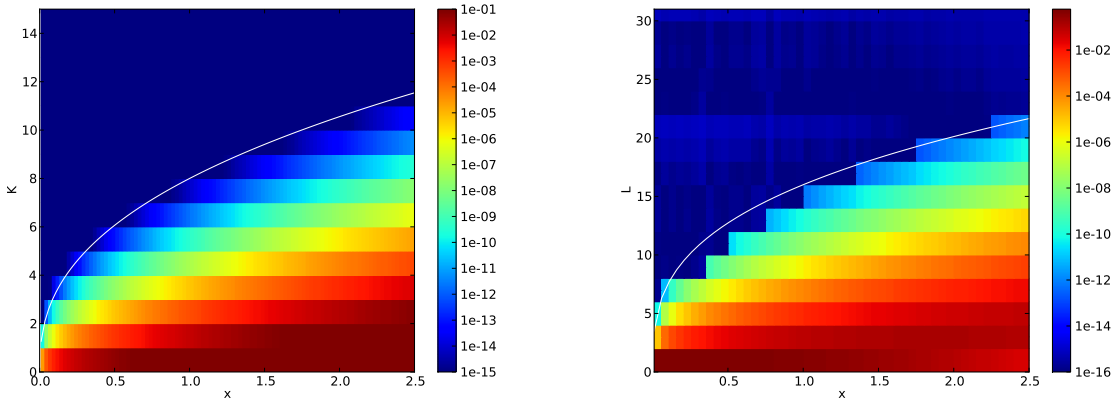

Figure 2. Left: Difference between the l.h.s. of (15) and unity as function of x and K. Right: l.h.s. of (18) as function of x and L. The white lines show the criteria (16) and (19), respectively.

kept. From this figure we can deduce the heuristic criterion

$$K \gtrsim 8 \cdot x^{2/5} \,. \tag{16}$$

In a similar way, we can derive a heuristic criterion for the minimum number of Legendre polynomials necessary to represent the QL diffusion coefficient. For this purpose, we note that due to the use of spherical velocity coordinates the integrand of Equation (7) contains the factor $(1-\mu^2)$, and thus vanishes at $\mu \pm 1$. However, since $P_n(\pm 1) = (\pm 1)^n$ for all n, convergence of the Legendre series to zero can be critically slow at these points (this is analogous to the Gibbs phenomenon of Fourier series). The worse situation is for $p = 0$, in which the expansion

$$(1-\mu^2)\; J_0^2(x\sqrt{1-\mu^2}) = \sum_{n=0}^{L=\infty} \left(n+\frac{1}{2}\right)\; P_n(\mu) \sum_{k=0}^{K=\infty} \mathcal{J}_{0,0}^k(x)\; \tilde{Q}_0^{(0,0)}(n,0,k) \tag{17}$$

becomes for $\mu = \pm 1$

$$\sum_{n=0}^{L=\infty} (\pm 1)^n \left(n+\frac{1}{2}\right) \sum_{k=0}^{K=\infty} \mathcal{J}_{0,0}^k(x)\; \tilde{Q}_0^{(0,0)}(n,0,k) = 0 \,. \tag{18}$$

From the identity (18) we can derive a criterion for the minimum number L of Legendre polynomials to be used in order to approximate the QL diffusion coefficient with a given numerical accuracy. Figure (2.right) shows the l.h.s. of Equation(18) as function of x and L; the number K of terms in the inner sum is chosen so as to satisfy the criterion (16). A rough rule of thumb to achieve double precision numerical accuracy is

$$L \gtrsim 16 \cdot x^{1/3} \,. \tag{19}$$

To gain a feeling of what the two criteria (16) and (19) imply for ICRF simulations, we can assume $\omega \approx p\; \Omega_{\rm ci}$ and $k_\perp \approx \omega / v_A$, with v_A the Alfvén speed: then $\xi_\perp \approx p\; 0.063\; \sqrt{n_i\; T_i}/B_0$, with n_i, B_0 and T_i respectively in 10^{19} m^{-3}, Tesla and keV. For typical plasma parameters, $\xi_\perp \approx p\; 0.1$. We conclude that to obtain an accurate Legendre representation of the quasilinear operator up to values of $v/v_{\rm thi}$ of a few tens, the number of Legendre polynomials and of the terms in (8) has to be of the order of a few tens. This is only a necessary condition to obtain

a well converged and positive-definite solution of the FP equation in the same velocity range. Experience shows that as soon as the heating rate is faster than the collisional relaxation the number of polynomials to be included exceeds the values foreseen by (19), and increases rapidly with increasing hf power per ion.

4. Toroidal effects in the zeroth–banana–width limit

In a tokamak the combination of the (nearly) horizontal gradient of the confining magnetic field B with the adiabatic invariance of the magnetic moment $\mu_b = mv_\perp^2/2B$ of the charged particles causes a toroidal modulation of their parallel velocity and the well-known trapping of a class of particles in the outer part of the device. Sufficiently deeply trapped ions have their turning point to the low-field side of the surface $\omega = p\Omega_c$, and do not see the resonance until diffused by collisions on a less deeply trapped orbit. To describe the effect of trapping in `SSFPQL`, the QL diffusion coefficient $D_p(v_\perp)$ has to be multiplied by a function describing its dependency on the velocity pitch-angle:

$$D_p(v_\perp;\psi) = D_0\; g\,(\mu;\psi)\,|J_{p-1}(\xi_\perp v_\perp) + \lambda_P\; J_{p+1}(\xi_\perp v_\perp)|^2 \tag{20}$$

(in reality g depends also weakly on the ion energy; to avoid an excessive slowing down of the execution time, however, in `SSFPQL` an average value has to be used). The function g approaches unity for well passing particles ($\mu \to \pm 1$), has a maximum for the value of μ characterizing ions which turn close to resonance, and thus spend more time interacting with the waves, and decreases rapidly to zero for smaller values of μ, i.e. for ions reflected before reaching the resonance. An example is shown in Figure (3.left). To include the factor g in the numerical

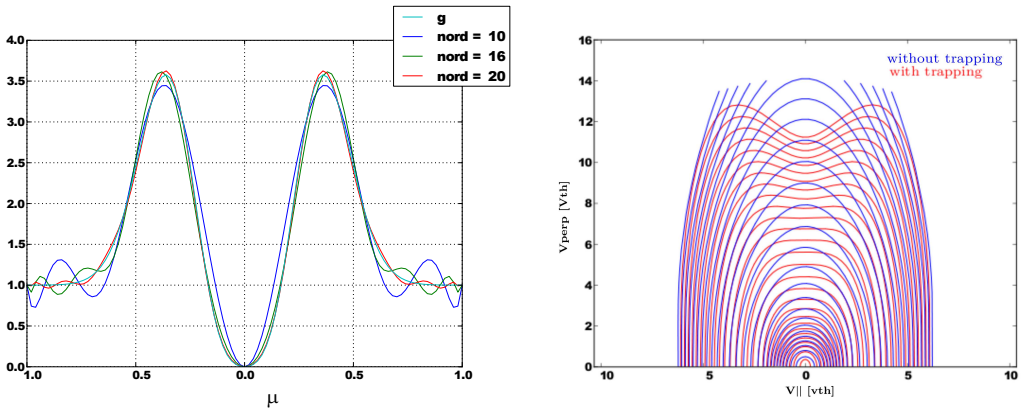

Figure 3. Left: Factor modeling trapping effects, and Lagrange-Chebyshev interpolants corresponding to three values of N_g. Right: Distribution function of hf heated species with and without trapping effects.

scheme of `SSFPQL`, we note that if g is approximated with a polynomial G_{N_g},

$$g(\mu;\psi) \simeq G_{N_g}(\mu) = \sum_{q=0}^{N_g} g_q(\psi)\; \mu^q\,, \tag{21}$$

the integrals X_p in Equation (12) become, for example,

$$X_p^{(g)}(n,m,k;\psi) = \sum_{q=0}^{N_g} g_q(\psi)\; X_p(n,m,k+q) \tag{22}$$

and similar expressions hold for Y_p and Z_p. It is sufficient, therefore, to evaluate the tables of these integrals without the factor g in the initialization phase of the run, and to use the convolution (21) with the appropriate function $g(\mu;\psi)$ to build the values needed on each magnetic surface ψ.

If the 'interpolant' polynomial G_{N_g} is looked for in the standard form (21), however, it is difficult to achieve a satisfactory accuracy. Instead, we use the Lagrange interpolant polynomial based on the set of $N_g + 1$ zeros of the Chebyshev polynomial $T_{N+1}(\mu)$ [12]. This minimize the Runge phenomenon, i.e. the tendency of the interpolant to oscillate between the base point with increasing amplitude towards the extremes of the interval of interpolation. Starting from the construction rules of the Lagrange interpolant, moreover, we have derived an efficient recurrence relation for the coefficients of G_{N_g} in the standard representation. Figure (3.left) shows three interpolants for three different values of N_g. The impact of the trapping effects on the solution of the FP equation is illustrated in Fig. (3.right). It is responsible for the characteristic rabbit-ears in the contour plot of the distribution functions, and for a reduction of number of fast ions produced by IC heating, an important issue for off-axis heating schemes.

5. Conclusion

We have discussed the control of truncation and round-off errors in the solution of the quasilinear kinetic equation based on the expansion in Legendre polynomials, and the extension of this technique in `SSFPQL` in order to take into account toroidal trapping effects in the limit of the zero–banana–width approximation. The extension of the interface between `TORIC` and `SSFPQL` to accept distribution functions modified by toroidal trapping is in progress.

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