Resonance frequency broadening of wave-particle interaction in tokamaks due to Alfvénic eigenmode

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Abstract

We use the guiding center code ORBIT to study the broadening of resonances and the parametric dependence of the resonance frequency broadening width $\Delta \Omega$ on the nonlinear particle trapping frequency $\omega_b$ of wave-particle interaction with specific examples using realistic equilibrium DIII-D shot 159243 (Collins et al 2016 Phys. Rev. Lett. 116 095001). When the mode amplitude is small, the pendulum approximation for energetic particle dynamics near the resonance is found to be applicable and the ratio of the resonance frequency width to the deeply trapped bounce frequency $\Delta \Omega / \omega_b$ equals 4, as predicted by theory. It is found that as the mode amplitude increases, the coefficient $a = \Delta \Omega / \omega_b$ becomes increasingly smaller because of the breaking down of the nonlinear pendulum approximation for the wave-particle interaction.

Keywords: resonance broadening, wave-particle interaction, RSAE, DIII-D

(Some figures may appear in colour only in the online journal)

1. Introduction

The confinement of energetic particles (EPs) is an important issue in present tokamaks and future fusion devices such as ITER limiting plasma operational regimes. EPs can drive shear Alfvénic gap modes and acoustic modes by releasing the free energy stored in the gradients of both real and velocity space. In turn, Alfvénic eigenmodes (AEs) can modify the EP distribution through wave-particle interaction (WPI). These instabilities can cause significant losses of heat and EPs, which then downgrades confinement and even damages the tokamak walls [1].

The resonance condition which describes the interaction of eigenmodes and particles is fundamental to the mode growth rate. According to the quasilinear theory, diffusion only occurs for the particles that exactly satisfy the resonance condition via a delta function [2]. However, the resonances are, in principle, broadened due to the finite growth rate and finite mode amplitude [3], and also effectively broadened due to stochastic processes affecting the resonant particles [4], such as collisions and microturbulence. Understanding the resonant broadened width of the WPI, affected by different dissipation mechanisms and nonlinear effects, can be crucial for the modeling of EP transport.

When mode overlapping occurs, which implies that the Chirikov criterion [5] is satisfied, then global diffusion of particles can occur. Particles move stochastically and therefore conventional quasilinear theory (CQL) [6, 7] provides a suitable description of the EP relaxation. We note, however, that the minimum stochasticization of phase-space required by
the CQL applicability can as well be provided by collisional and turbulent effects on resonant EPs. For the resonance overlapping situation, much of the fine phase-space structure of the distribution function is ‘averaged out’ due to particle decorrelation from a resonance. However, when individual resonances saturate at low levels without overlapping, they only perturb a localized portion of phase-space which does not lead to large-scale, global diffusion. In this case, particle redistribution can only occur within the resonance island because only the particles that are trapped by the wave undergo phase mixing. QL theory mimics the phase mixing by means of a diffusion coefficient that is not uniform in the phase-space, being non-zero only inside the resonance islands, where the distribution function is expected to be flattened. In addition, the particle diffusion due to a single mode is constrained to a one-dimensional manifold embedded in the full space.

Recently, DIII-D experiments observed that the fast ion transport induced by Alfvén eigenmode becomes stiff above a critical gradient. The results suggest that the threshold of AE-induced fast ion transport stiffness is above either the AE linear stability threshold or a microturbulent threshold [9]. To properly resolve transport in the velocity space, reduced models accounting for transport thresholds that differ in phase-space are required. Its details need to be studied using realistic parameter of the fusion experiments. Recently, a promising computationally efficient code RBQ1D [10] was built based on the resonance broadening description by earlier publications [4, 11]. It employs the resonance broadening quasilinear (RBQ) model [3] to study the EP transport including the diffusion coefficient and the mode amplitude self-consistent evolution with time. This reduced space dependence of the diffusion coefficient and the mode (RBQ) model [3] to study the EP transport including phase-space effects. In this work, we use the guiding center test particle modes and tearing modes, where the linear eigenmodes are not the poloidal mode number \(n\) but the poloidal angle, which can be estimated from a theoretical description or found more precisely using a numerical beam deposition code, such as NUBEAM routine of TRANSP [14]. Oscillations are prescribed through the following ansatz for the fluid displacement:

\[
\tilde{\xi} = \sum_{n,m} A_{nm}(\psi_p)e^{-in(\omega_n - m\sigma - \omega_n)t},
\]

where \(n\) refers to the toroidal mode number for a single mode with angular frequency \(\omega_n\) with several poloidal harmonics \(m\) and the amplitude \(A_{nm}\) is the magnitude of the ideal displacement caused by this mode. The Hamiltonian is a function of \(n\) \(\omega_n\) if there is only a single mode. Then we have

\[
\dot{P}_\zeta = -\frac{\partial H}{\partial \zeta} = n\dot{H}/\omega_n,
\]

and thus \(\dot{E} = E - \omega_n P_\zeta/n \approx \text{const}\) for a single mode (the value of the Hamiltonian is the energy \(E\)). The motion of particles in the \((E, P_\zeta)\) plane is therefore restricted to one dimension.

When the mode frequency is much lower than the cyclotron frequency \(\omega_c \ll \omega_r\), the wave-particle linear resonance condition is given by

\[
\Omega(E, P_\zeta, \mu) = n(\omega_n) - \langle \omega_R \rangle - \omega_n = 0,
\]

where \(l\) is an integer, \(\omega_c\) and \(\omega_R\) are the toroidal and poloidal transit frequencies and \(\langle \ldots \rangle\) denotes averaging over one poloidal transit time [11]. Note that in this expression the integer \(l\) is not the poloidal mode number \(m\). Usually the
integer $l$ is close to the poloidal mode number $m$ existing in the mode, but the exact resonance location can be only found by integrating over the particle poloidal trajectory [13].

Although the linear resonance condition implies that the equation (5) is only satisfied at singular points, there are effects that can naturally broaden the resonance, e.g. via nonlinear [4, 15] and collisional [16] mechanisms. The RBQ model [3, 11] was conceived as a modification of the usual quasilinear relaxation framework that copes with the expected single-mode saturation levels, as predicted by analytical theory. The RBQ employs the same structure of the quasilinear theory while considering that the resonances are broadened around a central point determined by the linear resonance condition in equation (5) [10]. The broadened resonance is the platform that allows momentum and energy exchange between particles and waves. It is assumed that the width of frequency broadening around resonance $\Omega = 0$ is [3]

$$\Delta \Omega = a\omega_b + b\gamma + c\nu_{\text{eff}}, \quad (6)$$

where $a$, $b$ and $c$ are coefficients, $\omega_b$ is the deeply-trapped particle bounce frequency of WPI, $\nu_{\text{eff}}$ is the effective scattering rate, and $\gamma$ is the linear net growth rate. The coefficients $a$ and $c$ in two extreme limits (far from and close to marginal stability) can be calculated analytically, respectively [4, 16–18].

In addition, the saturation level of toroidicity-induced Alfvén eigenmode (TAE) in TFTR of numerical simulation and the prediction from single wave saturation are in good agreement [19]. In this work, we study the resonance broadening due to a single mode to validate the coefficient $a$. A consistent study of mode saturation level to calculate coefficients $b$ and $c$ will be the scope of further work.

3. Numerical approach

In this work, we propose a numerical approach to measure the resonance broadening width and the trapping frequency. This method could in principle be used for detailed study of the distribution function modification due to WPI.

3.1. Equilibrium and mode

We use the parameters of the DIII-D discharge 159243 at 790ms. This case is described in Collins’ paper on the EP critical gradient model [9]. Figure 1 shows the equilibrium for this case. Other parameters are $B_0 = 19.77$ kG, major radius $R_0 = 172$ cm, minor radius $a = 63$ cm, $q_{\text{min}} = 2.95$ at $\psi_p = 0.24$.

To carry out simulations of realistic discharges, we use a mode structure and frequency determined by the ideal MHD code NOVA [20]. Collins did the work of comparing NOVA mode structure results with experimental electron cyclotron emission (ECE) data for all selected modes [21]. The chosen Reversed Shear Alfvénic Eigenmode (RSAE) near $q_{\text{min}}$ is critical to understand the EP transport leading to hollow EP pressure profiles, and yet the case we consider is nevertheless general to make conclusions for future RBQ development. The mode structure of this RSAE is shown in figure 2 with a single toroidal mode number $n = 4$ and frequency 82.03 kHz, with poloidal harmonics $m$ ranging from 11 to 23. The mode peaks at $\psi_p = 0.22$ near the $q_{\text{min}}$ and the dominant poloidal harmonic is $m = 12$. We use the largest value of the dominant poloidal component $m = 12$ as the mode amplitude $A = \delta B_r / B$.

3.2. NBI particle distribution

EP distributions are obtained from the beam deposition code NUBEAM in TRANSP [14]. This discharge 159243 is well studied and extensive efforts were undertaken by kick model
application and were recently published [22]. The distribution function is used in a forward-modeling code FIDASIM to predict fast-ion D-alpha (FIDA) and neutral particle analyzer (NPA) signals, and yields a calculated FIDA profile in excellent agreement with experiment, as shown in figure 12 in [22]. The distribution function \( f(E, \lambda) \) is integrated over the minor radius as shown in figure 3(a), which \( \lambda = v_{\parallel}/v \) is the pitch. This discharge had tangential co-injection and the injected energy is \( E_{\text{inj}} = 71 \) keV. Figure 3(b) shows the distribution in terms of the magnetic moment \( f(\mu B_0) \), which is integrated over the other coordinates. Without collisions, \( \mu \) is a constant for the guiding center equations used in ORBIT. We use \( \mu B_0 \) to convert the value of the magnetic moment to units of energy. The distribution \( f(\mu B_0) \) peaks at \( \mu B_0 = 20 \) keV, so we choose co-moving particles in the \((E, P_\perp, \mu B_0 = 20 \text{ keV})\) plane for detailed studies.

3.3. Wave-particle resonance

Linear wave-particle resonance \( \Omega = 0 \) can be calculated numerically by following particle trajectories in equilibrium, i.e., in the absence of a mode. The toroidal and poloidal transit frequencies \( \omega_t \) and \( \omega_p \) are calculated by following 50 000 particles and averaging the frequencies over about 10 poloidal transit times, in order to achieve reasonable accuracy. Then we use cubic interpolation to get a smooth resonance frequency plot of 200 000 points uniformly distributed on the \((E, P_\perp)\) plane. The interpolation is used to calculate \( \langle \omega_\perp \rangle \) and \( \langle \omega_p \rangle \) and then \( \Omega \) can be readily computed.

For calculating the resonance frequency, we first calculate \( (n\langle \omega_\perp \rangle - \omega_p)/\langle \omega_p \rangle \) to find the integer \( l \) on this \((E, P_\perp)\) plane, where \( l \) is the closest integer to \( (n\langle \omega_\perp \rangle - \omega_p)/\langle \omega_p \rangle \). As shown in figure 4(a), the colorbar value equals to \( \Omega/\omega_p \) and indicates the location of resonance. When \( \Omega/\omega_p = 0 \), linear resonance condition is satisfied and \( |\Omega/\omega_p| = 0.5 \) is far from resonance. Red lines are where the resonances conditions \( \Omega = 0 \) are satisfied with \( l = 9,10,11 \) and so on. For co-passing particles, \( \omega_\perp \approx q\omega_p \), the resonance lines have a turning point somewhere in \((E, P_\perp)\) plane for reversed \( q \) profile. This property can be clearly seen from the \( l = 9 \) resonance. For the \( l = 10 \) resonance, its turning point is at higher energy and outside the region \( 20 \text{ keV} < E < 70 \text{ keV} \) we studied. Even though there are many resonances near the trapped-passing separatrix, they do not contribute much to the growth rate.

The resonance lines show the linear resonance location in phase-space but they do not provide information on the resonance island width or on the strength of the local phase-space contribution to the growth rate, which is quite sensitive to the local distribution function. The phase vector rotation technique [23, 24] embedded in ORBIT code can be used to detect the broken Kolmogorov–Arnold–Moser (KAM) [25–27] surfaces efficiently and accurately in the presence of a single mode. The red points indicate the location of the broken KAM surfaces for a mode amplitude \( A = 1.5 \times 10^{-4} \). In figure 4(b) we can see that there is a dominant resonance near the right boundary, which corresponds to the magnetic axis. The dominant resonance is located near the largest mode amplitude, where the mode structure peaks.

3.4. Kinetic Poincaré plot

For more detailed study on the wave-particle resonance, a kinetic Poincaré plot can be employed to produce the high-resolution figures of the resonance island structure [13]. Contrary to the resonance condition plot figure 4(a), kinetic Poincaré plots are produced by following particle orbits in the presence of a mode with a single toroidal mode number and frequency, and recording points whenever \( n\zeta - \omega t = 2k\pi \) with \( k \) integer. In addition, when an island overlaps with other islands, the kinetic Poincaré plot become chaotic, which implies that the Chirikov criterion [5] is satisfied for this situation. The kinetic Poincaré plot shows the resonance only along the line \( E' = \) constant, with fixed magnetic moment \( \mu \). For studying the dominant resonance we are interested in, we choose four cases with \( E' = 30 \text{ keV}, 45.09 \text{ keV}, 51.93 \text{ keV}, 60.22 \text{ keV} \) intersecting with the dominant resonance lines, respectively. Their locations are the four parallel blue lines as shown in figure 4 from bottom to top. We will refer to them as Res 1,
4. Wave-particle trapping frequency

The trapping frequency $\omega_{tr}$ is the frequency of the bounce motion of a resonant particle trapped by the wave. It is a function of distance from the island O-point, dropping to zero at the separatrix. The deeply trapped bounce frequency $\omega_b$ is $\omega_{tr}$ at the O-point, which is proportional to the width of the island and to the square root of mode amplitude, $\omega_b \propto A^{1/2}$. The wave-particle trapping frequency for small amplitude oscillations, i.e. of a particle near O-point is given by [28]

$$\omega_{tr}^2 = \left\langle Z_{EPE}E \cdot \frac{n}{\omega} \frac{\partial \Omega}{\partial \psi} \bigg|_{\psi'} \right\rangle,$$

(7)

where $E$ is the electric field, $\mathbf{v}$ is the velocity, and the time average is taken for an exactly resonant particle.

We observe that the resonance islands are wide at the dominant resonance, where particle orbits intersect with the location of the mode peak as inferred from figure 4(b). Outside of this region, resonance islands are relatively narrow, which means small $\omega_b$. From Res 1 to Res 4, the resonance islands become increasingly stretched along the energy coordinate at the same mode amplitude, as inferred from figure 5. It implies that the deeply trapped bounce frequency $\omega_b$ is increasing, which can be seen from figure 12. The results show the $\omega_b$ is larger at the dominant resonance and high-energy regime.

The trapping frequency $\omega_{tr}$ is the angular frequency of a particle rotating $2\pi$ in the island as shown in the kinetic Poincaré plot. In this paper, we propose a numerical approach to calculate the trapping frequency and developed a MATLAB package for ORBIT data analysis. The trapping frequency of a particle is calculated numerically by following its orbit on the kinetic Poincaré plot. The details can be found in appendix.

4.1 Pendulum approximation

Since the resonance islands are stretched increasingly with increasing mode amplitude, highly asymmetric in $E$ direction, and particle orbits are stochastic near separatrix, it is hard to identify the island width accurately (see figure 14(b)). However, the resonance islands are nearly symmetric and do not stretch with mode amplitude in $\theta$ direction, so we choose $\Delta \theta$ as the variable to represent the distance from O-point. So we define the resonance island non-dimensional length in $\theta$ direction, which is an action angle. Then, the resonance island length is $L = 2\pi/l$ as shown in figures 6(a) and (b). The red rectangle is the resonance island chosen to calculate the trapping frequency.

For the case of a sinusoidal wave, the collisionless motion of the resonant particle around the O-point satisfies the pendulum equation [28]

$$\frac{d^2\alpha}{dt^2} + \omega_b^2 \sin(\alpha - \omega_b t - \alpha_0) = 0,$$

(8)

where $\alpha$ is the action angle and $\alpha_0$ is a constant phase.

$$\alpha = (n, -l, 0) \cdot (\zeta, \theta, \theta_c) = n\zeta - l\theta,$$

(9)
where \( n, -l, \) and \( \theta \) are the quantum numbers associated with the periodicity of the canonical angles \( \zeta, \theta \) and \( \theta_c \), the gyroangle, so the resonance frequency is \( \Omega = \dot{\alpha} - \omega_n \). Similarly to a pendulum, the energy-like variable of a trapped particle in the wave frame is

\[
E_{bt} = \frac{\dot{\alpha}^2}{2} + \omega_b^2 [1 - \cos(\alpha - \omega_b t - \alpha_0)] , \tag{10}
\]
where the first term and the second term represent the kinetic and the potential energies of the pendulum, respectively. The trapped particle energy ranges from 0 to $E_{bt} = 2\omega_b^2$, with $E_{bt} = 0$ at the O-point and $E_{bt} = 2\omega_b^2$ at the separatrix. The value of $a$ changes with time from $-\pi$ to $\pi$ when the particle orbit is at the separatrix, so we have

$$\dot{\alpha}^2/2 = \omega_b^2[1 + \cos(\alpha - \omega_b t - \alpha_0)] \leq 2\omega_b^2. \quad (11)$$

Therefore,

$$\Delta\Omega = \Omega_{\text{max}} - \Omega_{\text{min}} = 4\omega_b, \quad (12)$$

for trapped particles, which is the predicted resonance broadening width. Since, to the best of our knowledge, the factor 4 has not yet been checked in a realistic case, we perform a detailed study of the pendulum approximation in this paper.

The condition for a kinetic Poincaré plot is $n\zeta - \omega_b t = 2k\pi$. Substituting this condition and equation (9) into equation (8), then we have

$$-\frac{d^2(\theta)}{dt^2} + \omega_b^2 \sin(\theta + \alpha_0) = 0. \quad (13)$$

So we can derive the nonlinear trapping frequency when the pendulum approximation for the WPI is valid

$$\omega_{bt} = \omega_b \frac{\pi}{2} K(k), \quad (14)$$

where $K(k) = \int_\theta^\pi \frac{1}{\sqrt{1 - k^2 \sin^2 \phi}} d\phi$ is the first kind complete elliptic integral, $k = \sin(\frac{1}{2} \Delta\theta)$, $\Delta\theta = \Delta\theta/L$ is the normalized orbit length of a trapped particle and the angular range $\Delta\theta$ is indicated in figure 6(b). The deeply trapped bounce frequency is $\omega_b = \omega_{bt}(\Delta\theta = 0)$. Since the trapping frequency changes slowly in the island center, numerically we set $\omega_b$ equal to the trapping frequency of the particle with the minimal $\Delta\theta$.

Figure 6(b) presents the selected resonance island as shown in figure 6(a), which is ‘blown up’ by loading more particles in the resonance. The orbit of one particle is highlighted in red. We also plot its action angle $\theta$ changing with time in figure 6(c). The red star points are numerical data and the blue dots are interpolated points to improve the accuracy of fast Fourier transform (FFT). Then we use FFT to analyze the signal $\theta(t)$ to calculate the trapping frequency. The details can be found in appendix.

4.2. Numerical method to measure the resonance broadening

To calculate the resonance frequency broadening width $\Delta\Omega$, a new method is proposed to determine the broadening based on the linear distribution slope. $\Delta\Omega$ can be used to compute the broadening in $P_\xi$. As mentioned above, the resonance broadening region is the platform that allows momentum and energy exchange between particles and waves. So we can measure the broadening of energy distribution $\Delta\mathcal{E}$ from the relaxation results, then calculate the resonance frequency broadening width $\Delta\Omega$ according to the function $\Omega(\mathcal{E})|_{\mathcal{E}'}$. An example of this procedure is shown in figure 7. The EP relaxation in energy space is shown in figure 7(a). The initially loaded 40000 particles are divided into 80 bins, and the maximum number of particles in one bin is about 1000. The initial distribution of $\psi_p$ linearly decreases from 0.06 to 0.37, with $\theta_0 = 0$ and $\zeta_0$ being a random number. The initial distribution is almost linearly increasing in $P_\xi$ according to equation (2). And the distribution in energy is the same with in $P_\xi$ because $\mathcal{E}'$ is a constant. The total run time $T$ is about 3.89 ms with a fixed mode, much larger than the trapping time $T > \tau_b = 2\pi/\omega_b$. Usually the particle distribution oscillates near the island, since energy of particles near separatix oscillate with time. However, those oscillations do not contribute to the flattening. The relaxed distribution, shown in red line in the figure, is averaged over $\Delta t = 0.078$ ms $\ll \tau_b$ in order to remove these fluctuations. Figure 7(b) shows the dependence of $\Omega$ (defined by equation (5)) as a function of energy along the $P_\xi$ line. For this resonance, the resonance condition is $\Omega = 4(\omega_{\xi'}) - 10(\omega_b) - \omega_n$, $\omega_{\xi'} = 45.09$ keV. For this resonance, the maximum number of particles in one bin is about 1000. The initial distribution of $\psi_p$ linearly decreases from 0.06 to 0.37, with $\theta_0 = 0$ and $\zeta_0$ being a random number. The initial distribution is almost linearly increasing in $P_\xi$ according to equation (2). And the distribution in energy is the same with in $P_\xi$ because $\mathcal{E}'$ is a constant. The total run time $T$ is about 3.89 ms with a fixed mode, much larger than the trapping time $T > \tau_b = 2\pi/\omega_b$. Usually the particle distribution oscillates near the island, since energy of particles near separatix oscillate with time. However, those oscillations do not contribute to the flattening. The relaxed distribution, shown in red line in the figure, is averaged over $\Delta t = 0.078$ ms $\ll \tau_b$ in order to remove these fluctuations. Figure 7(b) shows the dependence of $\Omega$ (defined by equation (5)) as a function of energy along the $P_\xi$ line. For this resonance, the resonance condition is $\Omega = 4(\omega_{\xi'}) - 10(\omega_b) - \omega_n$. $\omega_{\xi'} = 45.09$ keV. For this resonance, the resonance condition is $\Omega = 4(\omega_{\xi'}) - 10(\omega_b) - \omega_n$.

5. Resonance broadening due to a single mode

5.1. Broadening coefficient $a = \Delta\Omega/\omega_b$ in realistic cases

Following this process, we study the resonance broadening with different mode amplitudes for four resonance Res 1 to 4, as shown in figures 8–11. The Res 1 case of figure 8 corresponds to particle initially loaded along the Res 1 line shown in figure 4. Figure 8(a) show the energy distribution change $\delta f = f(t = T) - f(t = 0)$ with different mode amplitudes, with $\delta f > 0$ on the left side of the island and $\delta f < 0$ on the right. On the right hand side...
of figure 8 shows the function $\Omega(E)|_{E=30}$ keV, the linear exactly resonant point $E_{\text{res}}$ is also pointed out, $E_{\text{res}} = 32.19$ keV. Figure 8(b) shows the comparison of numerical results of $a = \Delta\Omega/\omega_b$ with the theoretical prediction of pendulum approximation, $\Delta\Omega/\omega_b = 4$. When the mode amplitude $A < 5 \times 10^{-4}$, numerical results agree with the pendulum approximation. Other cases are represented the same way.

For Res 2, the linear resonant point is at $E_{\text{res}} = 51.1$ keV as shown in figure 9(a). When the mode amplitude $A < 5 \times 10^{-4}$, numerical result agrees with the pendulum approximation as shown in figure 9(b). For Res 3, the linear resonant point is at $E_{\text{res}} = 58.29$ keV as shown in figure 10(a). When the mode amplitude $A < 2.25 \times 10^{-4}$, numerical results agree with the pendulum approximation as shown in figure 10(b). For Res 4, the linear resonant point is at $E_{\text{res}} = 66.97$ keV as shown in figure 11(a). When the mode amplitude $A < 1.25 \times 10^{-4}$, numerical results agree with the pendulum approximation as shown in figure 11(b).

There are several similarities in these cases. The deeply trapped bounce frequency is almost proportional to the square root of the mode amplitude, $\omega_b \propto \sqrt{A}$, as shown in figure 12. It is found that the coefficient $a$ decreases as mode amplitude increases for these four cases, which indicates that the pendulum approximation breaks down. For Res 3 and Res 4, the pendulum approximation breaks down at lower mode amplitude in comparison with Res 1 and 2. This is because that at the same mode amplitude, the island width and the deeply trapped bounce frequency are larger for these four cases as shown in figures 5 and 12. It is also found that the pendulum approximation breaks down at $\omega_b$ around 30 rad ms$^{-1}$ from figures 8(b)–11(b).

It is found that the platform center does not move significantly for Res 1 case. The derivative $\partial \Omega/\partial E$ is roughly the same at $E < E_{\text{res}}$ and $E > E_{\text{res}}$. For Res 2, 3 and 4 cases, the platform center moves to the left significantly and the energy broadening $\Delta E$ does not increase equally on each side. The derivative $\partial \Omega/\partial E$ is smaller at the $E < E_{\text{res}}$ region. So the resonance islands of Res 2, 3 and 4 are highly asymmetric compared to Res 1 as shown in figure 5, and the broadening in energy is larger at $E < E_{\text{res}}$. 

Figure 8. Res 1 case. (a): Energy distribution change $\delta f$ and $\Omega(E)|_{E=30}$ keV, (b): $\Delta\Omega$ variation with $\omega_b$. The value $5 \times 10^{-4}$ shown in the plot corresponds to the amplitude at the break down of the pendulum approximation.

Figure 9. Res 2 case. (a): Energy distribution change $\delta f$ and $\Omega(E)|_{E=40}$ keV, (b): $\Delta\Omega$ variation with $\omega_b$. The value $5 \times 10^{-4}$ shown in the plot corresponds to the amplitude at the break down of the pendulum approximation.
5.2. Pendulum approximation viability for realistic cases

As mentioned above, the pendulum approximation works very well up to a certain point of the mode amplitude in realistic cases. It is found that $a$ is getting increasingly smaller than 4 as the mode amplitude increases, and the pendulum prediction of the coefficient $a$ breaks down at smaller mode amplitude for Res 3 compared to Res 1. So we investigate the pendulum approximation at Res 1 and Res 3, as shown in figure 13.

The solid lines in figures 13(a) and (c) are fitting curves using equation (14), with the $\omega_b$ set as the numerical trapping frequency of particle with the minimal $\Delta \theta$, and points are trapping frequencies calculated numerically. Some points are vertically aligned at the same $\Delta \theta$ near the right edge because of the particle stochastic motion at the separatrix. For Res 1, the particle trapping frequency $\omega_b$ agrees with the theory as shown in figure 13(a), and $a = \Delta \Omega / \omega_b \approx 4$ as shown in figure 13(b) up to mode amplitude $A = 5 \times 10^{-4}$. For Res 3, when the mode amplitude $A = 3.25 \times 10^{-4}$, it can be clearly seen that the trapping frequency deviates from the pendulum approximation at Res 3 case. 

$\Delta \Omega = 4 \omega_b$

The value $2.25 \times 10^{-4}$ shown in the plot corresponds to the amplitude at the break down of the pendulum approximation.

$\Delta \Omega = 4 \omega_b$

The value $1.25 \times 10^{-4}$ shown in the plot corresponds to the amplitude at the break down of the pendulum approximation.

$\Delta \Omega = 4 \omega_b$

The value $2.25 \times 10^{-4}$ shown in the plot corresponds to the amplitude at the break down of the pendulum approximation.

$\omega_b$ variation with mode amplitude $A$ at four cases. Dots are numerical data and dashed line are fitting results. At the same mode amplitude, the deeply trapped bounce frequency $\omega_b$ is increasing from Res 1 to 4.
approximation as shown in figure 13(c). When the mode amplitude $A = 7.5 \times 10^{-4}$, the numerical trapping frequencies do not show a regular pattern when $\Delta \theta > 0.3$ because particle orbits become chaotic in that regime.

We observe that the trapping frequency is always below the theory predicted by equation (7), e.g. when the mode amplitude $A = 3.25 \times 10^{-4}$ at Res 3. It is found that the resonance island is highly asymmetric in this case, as shown in figure 14(b). When the mode amplitude is large, e.g. $A = 10^{-3}$, the separatrix no longer exists and becomes a band of chaotic trajectories with nonzero thickness as shown in figure 14(c).

Equation (8) describes an exact pendulum and gives rise to an exactly defined separatrix between the island interior and the topologically unperturbed exterior. However, for the realistic cases, the amplitude of the wave trapping well is related with the poloidal flux, i.e. the wave is non-sinusoidal, the WPI term in equation (8) is no longer sinusoidal function with a constant amplitude $\omega_0^2$. In addition, there is not only one resonance and other resonances will give an additional perturbation term to equation (8). Then the trapped particle motion can become highly nonlinear and more complicated [13]

$$\frac{d^2 \alpha}{dt^2} + V(\psi_p) \sin(\alpha - \omega_p t - \phi_0) + \epsilon \sin(j \alpha - \omega_p t - \phi_0) = 0. \tag{15}$$

When the mode amplitude becomes large, the resonance island becomes too wide and the eigenmode structure is varying within the resonance island so using a constant $V$ is not a good approximation anymore. The third term of equation (15) accounts for small high-order oscillations, with $j$ an integer. In principle, we can find the deviation of the trapping frequency and estimate the thickness of the chaos band.

Figure 13. (a) and (c): Trapping frequency variation with $\Delta \theta$. Solid lines are fitting curves from the analytical prediction shown in equation (14), points are trapping frequencies calculated numerically. (b) and (d): Coefficient $a = \Delta \Omega/\omega_0$ variation with different mode amplitudes $A$. Figures (a) and (b) are for Res 1 ($l = 9$): particle trapping frequency $\omega_0$ agrees with theory, and $a \approx 4$ for all mode amplitudes. Figures (c) and (d) are for Res 3, ($l = 10$): $a$ decreases with mode amplitude $A$. When $A \geq 3.25 \times 10^{-4}$, the pendulum approximation breaks down substantially.
However, there are no analytic representations for $V(\mathcal{E})$ and $\epsilon \sin(j_0 \omega t - \varphi_0)$.

We choose three representative mode amplitudes of the Res 3 case and plot the resonance islands to discuss the process and reasons of pendulum approximation breakdown: at $A = 2.5 \times 10^{-5}$, numerical trapping frequency $\omega_{bt}(\Delta \theta)$ agrees with pendulum prediction in equation (14); at $A = 5 \times 10^{-4}$, $\omega_{bt}(\Delta \theta)$ drops below the prediction; at $A = 1 \times 10^{-3}$, $\omega_{bt}(\Delta \theta)$ is irregular, as shown in figure 13(c). We observe that the trapping frequency shifts down with respect to the theory first due to the resonance island deformation, then the particle orbit becomes stochastic at large mode amplitude as shown in figure 14. When the mode amplitude is small, $A = 2.5 \times 10^{-5}$, the resonance island shape looks like the exact pendulum as shown in figure 14(a). As the mode amplitude increases, $A = 5 \times 10^{-4}$, the resonance island deforms and stretches along the $\mathcal{E}$ direction as shown in figure 14(b). When the mode amplitude $A = 1 \times 10^{-3}$, significant chaos occurs as shown in figure 14(c). Particle orbits near the ‘separatrix’ become a thick chaos band, as an example, one particle orbit is highlighted in green. Actually, there is no defined ‘separatrix’ because there are always a series of higher-order perturbed terms in the Hamiltonian due to the complexity of the realistic equilibrium. But at small mode amplitude, the perturbed Hamiltonian can be neglected and the chaos band is very narrow. In addition, an example of particle orbit change due to higher order resonance is highlighted in red. The linear $l = 10$ island is surrounded by 4 small islands, which means $l = 40$ of this higher order resonance. Another particle orbit is highlighted in blue with $l = 70$. These high order perturbations have an important effect on trapped particle motion when the mode amplitude is large.

5.3. Averaging in constant of motion phase-space

When the mode amplitude is small, the coefficient $a = 4$ is a good choice to compute the resonance line broadening. When the mode amplitude becomes larger, the coefficient is observed in the simulation to be smaller than 4 and dependent on the resonance location in the COM phase space. As inferred from figures 8(b)–11(b), figures 4(b) and 13, the pendulum approximation breaks down at the dominant resonance (at the position of largest perturbation) and higher energy regime of phase-space when the mode amplitude $A = 5 \times 10^{-4}$ but still works well at a large domain where the resonance islands are narrow, which means small $\omega_{bt}$. Figures 5 and 12 show that, for the case of a fixed mode amplitude, the resonant islands become broader for larger resonant energies, meaning that also the bounce frequency should increase, which is consistent with expression equation (7). Complementary to the energy dependence of the bounce frequency of the deeply-trapped particles, we see from figure 13 that, for a given mode amplitude, the pendulum approximation is observed to be poorer for higher resonant energies. In addition to the nonlinear dynamics dependence on the energy, we also examined the effect of the eigenstructure. We show in figure 4 the curve (in dashed black line) representing the peak of the mode structure, which represents particle orbit passing through $(\psi_p = 0.22, \theta = 0)$ point. We note that the bounce frequency equation (7), through its dependence on the electric field, is also sensitive to the radial spread of the mode, being larger for cases in which the resonance location is closer to the mode structure peaks location. Since we are aiming to find the universal coefficients, the averaging of broadening coefficients in the COM phase-space is recommended [19, 29].

$$\bar{\pi} = \int aQd\Gamma / \int Qd\Gamma$$  \hspace{1cm} (16)

where $d\Gamma$ is the differential phase-space volume, $Q \sim \xi_0^3 \delta(\Omega) \sim \omega_{bt}^3 \delta(\Omega)$, the $\delta$ function gives the integration along the resonance curve.

6. Summary

In this work, we study the resonance broadening due to a single wave in a realistic DIII-D plasma. We propose a numerical approach to measure the width of the resonance for the distribution function flattening and to calculate the corresponding resonance broadening $\Delta \Omega$. The evolution of the distribution function is obtained by using the guiding center, test particle code ORBIT for DIII-D discharge 159243. In principle, this method can be employed in different codes to measure the
resonance broadening for cases in which the resonant particle relaxation is known. We also propose a numerical technique and develop a MATLAB package to find the trapped particles and calculate the trapping frequency corresponding to WPI. This method can in general be used in different codes for analyses of both configuration-space (such as Poincaré plots of magnetic islands) and phase-space island properties.

Our work studies the validity of WPI in tokamaks being formally described as a nonlinear pendulum. It is found that when the mode amplitude is small, the nonlinear pendulum approximation is applicable and the coefficient $\Delta \Omega/\omega_p$ equals to 4 as analytically predicted (in section 4). As the mode amplitude increases, the resonance island deforms, and then significant chaos takes place, bringing the realistic case gradually away from the pendulum approximation validity. It is found that the trapping frequency drops down faster than the theory predicts. Consequently, the calculated coefficient becomes smaller than 4.

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**Appendix**

We propose a numerical method to calculate the trapping frequency and developed a MATLAB package for ORBIT kinetic Poincaré plot data analysis. This method is general for particle orbit classification and trapping frequency calculation and can be used for data analysis for other codes.

**A.1. Search for resonance island**

To get a high-resolution kinetic Poincaré of the resonance island for calculating the trapping frequency changing with $\Delta \theta$, the first step is to give initial particle guiding center coordinates $(\psi_p, \theta, \zeta, \rho_p)$ and to load the particles uniformly inside the resonance island. For the sake of simplicity, the following approach is adopted. The first step is to use the resonance frequency plot figure 4(a) or the phase vector rotation plot figure 4(b) to first roughly find the resonance location $(\mathcal{E}, \mathcal{P}_c)$. In principle, the $(\psi_p, \theta, \rho_p)$ can be calculated accordingly. However there are no analytic equations to obtain them easily since $B(\psi_p, \theta)$ is not prescribed analytically, so we load particles uniformly in $(\psi_{p1}, \psi_{p2})$ instead of loading particles uniformly on the line of $(\mathcal{E}, \mathcal{P}_c)$ with constant $\mathcal{E}$’ with initial poloidal angle $\theta = 0$. Choosing $\theta$ does not restrict the mode-particle phase since the toroidal angle $\zeta$ is a random number from 0 to $2\pi$ [13]. Now we just need to find the $(\psi_{p1}, \psi_{p2})$ of the resonance. In equilibrium, particle orbits which pass through the $(\psi_p, \theta = 0)$ point satisfy

$$\frac{((P_c + \psi_p)B(\psi_p, 0))^2}{2g(\psi_p)^2} + \mu B(\psi_p, 0) - \mathcal{E} = 0.$$  
(A.1)

It is a parabola on the $(\mathcal{E}, \mathcal{P}_c)$ plane, similar to the magnetic axis line as shown in figure 4. Therefore we can find the $(\psi_{p1}, \psi_{p2})$ corresponding to the resonance. We load 300 particles uniformly in a range of $0.04\psi_w$, which is enough to show details of the resonance island structure.

**A.2. Particle orbit classification**

Usually the resonance island is highly asymmetric in $\mathcal{E}$ direction but nearly symmetric in $\theta$ direction, so we choose $\Delta \theta$ as the variable to represent the distance from the O-point. We select one resonance island in the island chains on the Poincaré plots by selecting the points only in a region of $\theta$. The boundary is set at two X-points $[\theta_L, \theta_U]$ by hand. The selected $\theta$ range is slightly smaller than the island length, $\theta_U - \theta_L \approx 2\pi/l$. Then we compute the orbit length $\Delta \theta$ and width $W_b = E_{\text{max}} - E_{\text{min}}$ of every particle. Note that, there are always some passing particle orbits near the resonance island as shown in figure 6(b), their $\Delta \theta$ always equals to the $\theta_U - \theta_L$. Using $\Delta \theta$ one cannot tell how far from O-point a passing particle is. The pseudo trapping frequency of these passing particles will give some points vertically aligned at $\Delta \theta = \theta_U - \theta_L$. So we find a way to classify the particle orbit type to be either trapped or passing.

A particle with the smallest $\Delta \theta$ is marked as the most deeply trapped particle, which gives $\omega_p$. A particle with $\Delta \theta \leq 0.95(\theta_U - \theta_L)$ is identified as trapped, then we need to classify the passing and trapped particles near separatrix. The particle which has the maximum energy change, i.e. the largest orbit width $W_{bO}$, is at separatrix. The width of its trajectory in $(\mathcal{E}, \theta)$ space is identified as the separatrix width $W_{Sp}$. Then particles with $W_{bO} > 0.95W_{Sp}$ are identified as trapped ones to find the trapped particle with $\Delta \theta > 0.95(\theta_U - \theta_L)$. All the others are identified as passing.

**A.3. Trapping frequency calculation**

The action angle $\theta$ change with time for a trapped particle is basically sinusoidal plus a noise level. We use Fast Fourier Transform (FFT) to calculate the trapping frequency automatically. It can find the dominant frequency of the signal $\theta(t)$, which is the trapping frequency of the particle, which thus improves the robustness of this method when the action angle boundaries $[\theta_L, \theta_U]$ are not selected accurately and when the particle orbit is influenced by higher order resonances. The run time is chosen to be about $T = 10\text{ms}$. The number of sampling points of the signal data is about 500, which are
interpolated to 2048. The FFT calculates discrete frequency with accuracy proportional to \(1/T\). In order to smooth out aliasing errors, the following Gaussian filter is also adapted

\[
F_G = \frac{1}{\sqrt{\pi} T_G \text{erf}(\frac{x}{2T_G})} \exp \left[ -\left( \frac{t - T/2}{T_G} \right)^2 \right]. \tag{A.2}
\]

where \(\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\tau^2} \, d\tau\) is the error function. The \(T_G\) of the Gaussian filter is chosen as \(T_G = T/4\), which is much larger than the bounce period \(\tau_B\). The trapping frequency is calculated from the weighted mean value of frequencies corresponding to the proper amount of the dominant Fourier components. When particle moves stochastically such as at the separatrix, the numerical trapping frequency varies because the signal \(\theta(t)\) will include points actually from up and down resonance islands and increase the numerical trapping frequency as shown in figures 13(a) and (c).

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