

Magnetic Field Line Diffusion at the Onset of Stochasticity

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Dedicated to Professor Dieter Pfirsch on his 60th Birthday

The Hamiltonian equations of a particle in a random set of waves just above the stochasticity threshold are considered both theoretically and numerically. First we derive the diffusion coefficient and the autocorrelation time perturbatively without using the thermodynamic limit, and we discuss the relevance of the Hamiltonian problem for particle acceleration and magnetic field line flow. Then we integrate the equations for an ensemble of magnetic field lines numerically for a model problem [15] and show the time evolution of moments and correlations. Twice above the threshold we observe diffusive behaviour from the beginning, but the diffusion coefficient includes also the non-resonant modes. Just at threshold we find first a short phase of free acceleration, later a diffusion which is slower than predicted by the theoretical formula. The best way to analyze the problem is in terms of cumulants, but a reliable comparison with any theory requires also a time integration of the corresponding kinetic equations.

1. Introduction

Since the early days of quasilinear theory [1, 2] many attempts have been made to understand quantitatively the behaviour of turbulent plasmas. Here the turbulence problem seemed to be more accessible for analytical methods than ordinary hydrodynamic turbulence due to the presence of wave motions [3] and an associated smallness parameter. Several attempts to improve the earliest perturbative treatments are known as “weak turbulence”, “resonance broadening”, “direct interaction approximation” or “diffusion with memory effects”, and are mostly similar to methods which are also used in other fields of theoretical physics. To make further progress one could hope that either physical or computer experiments would lead to a general agreement on the “best” or “most valid” theoretical description of plasma turbulence, but this has not been possible so far. In order to facilitate the comparison between theory and numerical experiments, several authors studied numerically the trajectories of particles in prescribed “random” fields, thus avoiding the complexity introduced by the self-consistent evolution of fields and particle distributions [4–6]. The general result of these studies can be described as follows: While the quasilinear description (Fokker-Planck equation for the velocity distribution

function of the particles) is valid in a certain parameter range, there is another range – larger field amplitudes, longer evolution time – where not only the quasilinear theory fails, but also its “improvements” mentioned above.

Long ago it has been recognized that a Hamiltonian system may exhibit a diffusive behaviour if the interaction energy consists of a sufficiently dense set of resonant waves with sufficiently high amplitudes [7, 8]. This “overlap reasoning” has been verified by many numerical studies of mapping equations (e.g. [9–14]); it has also been verified recently in the study of a Hamiltonian problem which models continuous stochastic magnetic field lines of a plasma torus [15]. Here, however, a dramatic loss of numerical accuracy was observed as soon as the fluctuation level was slightly above the stochasticity threshold, and the numerical uncertainty increased with increasing fluctuation amplitudes and increasing evolution time. This numerical instability seems to be unavoidable for chaotic systems, but it cannot be detected in mapping equations where usually one iteration corresponds to a macroscopic step size. On the other hand, the progression of numerical errors has also been studied for several maps [16, 17] with the result that the time average of a function $f(\mathbf{x})$ along an orbit $\mathbf{x}(t)$ may be rather insensitive against artificially included errors of the map if the orbit is sufficiently long (ca. 10^5 iterations). This mainly empirical fact is rather astonishing since a

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numerically determined pseudo-orbit “depends essentially on the numerical method and even on the machine used, so that at first sight one could think that it has no meaning” (p. 185 of [16]). In approximating a continuous trajectory, the situation is worse: We cannot reach these asymptotic times so easily, and the numerical instability may affect all results more seriously, not only the trajectory itself. Therefore, we reconsider the overlap between quasilinear theory and numerical experiment for short times; in particular, we are interested in the case where the wave amplitudes are small enough to allow a perturbative treatment, but large enough to destroy the local KAM surfaces of resonances. In [15] it was observed that the numerical diffusion of the phase of the “particles” was much faster than the diffusion of the action variable; so one can expect that ensemble averages with respect to the phase of particles or waves at some initial time will later be numerically more stable than individual quantities. Moreover, it is not clear how far above the stochasticity threshold a system must be before the quasilinear diffusion is possible: In the “standard map” the quasilinear limit is only approached at a very large amplitude of the wave [12]; in [4] and [5] only an averaged overlap condition was considered, and in [5] its existence could even not be verified numerically. A further difficulty arises from the velocity-dependence of the quasilinear diffusion coefficient: It can be “measured” numerically from the time dependence of the velocity variance for a short initial time because one starts always with the same particle velocity; but later on the distribution of velocities becomes gradually broader due to the diffusion process, and the choice of the initial time interval where a straight line is fitted seems to be rather arbitrary. This difficulty cannot be avoided, too, by extrapolating the numerically determined diffusion coefficient at time t to $t \rightarrow \infty$ [18]. Finally, the theoretical description always assumes the “thermodynamic limit”, i.e. an infinite period in space and time; this leads to an unambiguous definition of the Lagrangian autocorrelation time which a particle experiences along an unperturbed orbit – but only for the theory, not for the computer model. Up to now the ambiguity of defining a Lagrangian autocorrelation time for discrete modes has been resolved only in a trivial fashion, i.e. one replaces the

quasilinear integral by a discretized approximation. Yet it is also of practical interest to know the effect of relatively few modes with not too large mode numbers, e.g. in the problem of field line diffusion: Only these modes can experimentally be detected.

Therefore, we present in Sect. 2 the Hamiltonian problem in action-angle variables for a system of one degree of freedom in a periodically time-dependent external field without resorting to the thermodynamic limit. First we quote the critical amplitudes for stochasticity, then we derive expressions for the diffusion coefficient and the autocorrelation time as functions of an averaging time Δt which remains an open parameter. In Sect. 3 we discuss two examples which fit into this frame: The acceleration of particles by a set of random waves, and the model for tracing magnetic field lines which was used in [15]. The thermodynamic limit for the first example is explained in the appendix. Section 4 gives typical numerical results for the second example: We show the first two moments and the second cumulant of the action variables as functions of time; the latter quantity is the best indicator of a diffusion process. Finally, we show the theoretical diffusion coefficient for several values of Δt and the action variable and compare it with the numerical results. A more detailed description of the numerical procedure and its application to the first example will be given elsewhere [19].

2. The Hamiltonian Problem

We consider a Hamiltonian in action/angle variables (J, θ) of the following form:

$$H = H_0(J) + H_1(J, \theta, t),$$

where the interaction energy H_1 is assumed to be periodic in the angle θ and time t , with period 2π in both cases. The “unperturbed trajectories” are the solutions of the integrable problem with $H_1 = 0$, namely:

$$J = \text{const}; \quad \theta(t) = \text{const} + \omega(J)t \quad (1)$$

with

$$\omega(J) = \frac{dH_0}{dJ} = \text{const}.$$

Interpreting (J, θ) as polar coordinates in a particular phase space, we obtain the continuous version of Moser’s “twist map”: Any representa-

tive point with initial coordinates (J_0, θ_0) rotates on the circle $J = J_0$ with constant angular velocity $\omega(J_0)$. The general behaviour of the trajectories for finite H_1 is a delicate question; while the famous KAM theorem asserts that for sufficiently small interaction energy – and some conditions which are usually physically acceptable – the trajectories are still confined between closed orbits, we know from experience with numerical solutions that for increasing H_1 an increasing area of phase space is accessible for “chaotic” trajectories. Fortunately, the transition region appears usually in the regime of “weak interaction” which is accessible both to analytical (perturbative) and numerical treatment. In this section we summarize the usual perturbative reasoning and discuss its results.

The first step is a Fourier representation of the interaction energy with mode numbers (m, n) (integers) running from $-\infty$ to $+\infty$:

$$H_1(J, \theta, t) = \sum_{m, n} H_{mn}(J) \exp[i(m\theta - nt)],$$

requiring the usual reality condition (the star denotes the complex conjugate):

$$H_{-m-n} = H_{mn}^*.$$

A particular mode (m, n) is said to be resonant if its phase $(m\theta - nt)$ is constant in time according to the unperturbed motion as given by (1). Thus we obtain the resonance condition which selects a particular unperturbed trajectory $J = J_{mn} = \text{const}$:

$$\alpha_{mn}(J) \equiv m\omega(J) - n = 0. \quad (2)$$

Another resonant mode (m', n') may select another trajectory $J = J_{m'n'}$, and the frequency distance between both resonances is then

$$\delta\omega = \left| \omega(J_{mn}) - \omega(J_{m'n'}) \right| = \left| \frac{n}{m} - \frac{n'}{m'} \right|.$$

A local condition for the true trajectory to be stochastic near the curve $J = J_{mn}$ is provided by the overlap criterion [8] whose evaluation, however, depends on some details.

Several more elaborate methods to estimate the critical parameters for the disappearance of KAM-surfaces have been developed [11, 20], but we will use the Chirikov-criterion because it results in a simple analytical formula. Considering the region of phase space, where

$$0 < \omega(J) < 1, \quad (3)$$

and requiring that only “neighbouring” mode numbers with $|n' - n| \leq 1$, $|m' - m| \leq 1$ have to be considered, one finds (compare [21] with appropriate changes in notation):

$$2|H_{mn}| \geq 2|H_{mn}|_{\text{crit}} \equiv \left[\frac{\Gamma}{4(m+1)} \right]^2 \cdot |\omega'_{mn}|^{-1} \cdot \text{Min}[\omega_{mn}^2, (1 - \omega_{mn})^2] \quad (4)$$

with

$$\omega_{mn} = \omega(J_{mn}) = n/m; \quad \omega'_{mn} = \left. \frac{d\omega}{dJ} \right|_{J=J_{mn}}.$$

Here, Γ is a number of order 1 (stochasticity parameter) whose exact value depends on the particular model. If the interaction energy contains only one basic frequency n we have the constraint $n' = n$, and the result is again (4) with the following replacement:

$$\text{Min}[\omega_{mn}^2, (1 - \omega_{mn})^2] \rightarrow \omega_{mn}^2. \quad (5)$$

The condition (4) shows that an appreciable area of phase space may be filled with stochastic trajectories without violating the condition of weak interaction, $|H_1| \ll |H_0|$, provided the shear parameter $|\omega'_{mn}|$ is large enough; this can also be true if the mode numbers m are not larger than 1.

In a second step we study the short-time behaviour of an ensemble of trajectories starting with the same initial values $\theta = \theta_0$ and $J = J_0$ at $t = 0$, but with randomly distributed initial phases of H_{mn} . We integrate the equation of motion for J individually over a time interval Δt which is short enough so that the total time dependence of H_1 is again obtained by the unperturbed trajectories, (1):

$$\frac{dJ}{dt} = - \frac{\partial H}{\partial \theta} = \sum_{m, n} c_{mn} \exp(i\alpha_{mn}t). \quad (6)$$

Here, α_{mn} is given by the left part of (2) with $J = J_0$, and

$$c_{mn} = -imH_{mn}(J_0)e^{im\theta_0}.$$

Denoting the statistical averages of the c_{mn} 's with respect to the phases of H_{mn} by brackets $\langle \rangle$ we calculate the diffusion coefficient $\langle (\Delta J)^2 \rangle / 2\Delta t$ as a function of Δt and J_0 , with $\Delta J = J(\Delta t) - J_0$:

$$\begin{aligned}
D(\Delta t, J_0) &\equiv \langle (\Delta J)^2 \rangle / 2 \Delta t \\
&= \sum_{m,n} \sum_{p,q} \langle c_{mn} c_{pq}^* \rangle (\exp\{i\alpha_{mn}\Delta t\} - 1) \\
&\quad \cdot (\exp\{-i\alpha_{pq}\Delta t\} - 1) / (\alpha_{mn} \alpha_{pq} \cdot 2 \Delta t).
\end{aligned}$$

Since the phases of the c 's are taken at the initial time $t = 0$ we can assume that they are independent; by this way we assume that J is driven by a set of turbulent waves whose two-point correlation corresponds to homogeneous statistics in space and time, as we shall see in a moment. Therefore, we have (using the Kronecker δ 's):

$$\langle c_{mn} c_{pq}^* \rangle = |c_{mn}|^2 \delta_{m,p} \delta_{n,q}, \quad (7)$$

$$\text{and} \quad D(\Delta t, J_0) = \sum_{m,n} \left| \frac{c_{mn}}{\alpha_{mn}} \right|^2 \cdot \frac{1 - \cos(\alpha_{mn} \Delta t)}{\Delta t}. \quad (8)$$

$$= \sum_{m,n} |c_{mn}|^2 \cdot \frac{2 \sin^2(\alpha_{mn} \Delta t / 2)}{(\alpha_{mn})^2 \Delta t}. \quad (8')$$

The last factor in (8') plays the role of the Dirac δ -function in quasilinear theory, as is shown in the appendix. It is well known that the quasilinear description not only requires small perturbation energy, but also a small Lagrangian autocorrelation time τ_{ac} . To derive an expression for this quantity we start again from the equation of motion for J :

$$\begin{aligned}
\frac{dJ}{dt} &= - \frac{\partial H}{\partial \theta} \equiv a(\theta, t) \\
&= \sum_{m,n} (-im H_{mn}) e^{i(m\theta - nt)}. \quad (9)
\end{aligned}$$

The independence of the phases of H_{mn} leads then to the following two-point correlation:

$$\begin{aligned}
\langle a(\theta, t) a(\theta', t') \rangle \\
= \sum_{m,n} |m H_{mn}|^2 \exp[i m(\theta - \theta') - i n(t - t')]. \quad (10)
\end{aligned}$$

Here we see first that only the differences of the arguments of the a 's enter corresponding to homogeneity in space and time as stated above. The Lagrangian autocorrelation time which the system experiences along an unperturbed orbit during a time Δt is then given by

$$\begin{aligned}
\tau_{ac}(\Delta t) &= \varepsilon^{-2} \int_0^{\Delta t} dt \langle a(\theta(t), t) a(0, 0) \rangle \\
&= \varepsilon^{-2} \sum_{m,n} |m H_{mn}(J_0)|^2 \frac{\sin(\alpha_{m,n} \Delta t)}{\alpha_{m,n}} \quad (11)
\end{aligned}$$

with

$$\varepsilon^2 \equiv \langle a^2 \rangle = \sum_{m,n} |m H_{mn}(J_0)|^2 = \sum_{m,n} |c_{mn}|^2.$$

Obviously, no definit limit of τ_{ac} is approached when $\Delta t \rightarrow \infty$, therefore, the diffusive nature of the ensemble of trajectories remains questionable. However, we can derive the following relation from (8) and (11):

$$\frac{\partial}{\partial \Delta t} [\Delta t D(\Delta t, J_0)] = \varepsilon^2 \tau_{ac}(\Delta t).$$

From (8) it is clear that $D(\Delta t, J_0)$ is zero for $\Delta t \rightarrow 0$ and $\Delta t \rightarrow \infty$; therefore, we find at least one value of Δt where the derivative of D with respect to Δt vanishes. If it vanishes for the first time at $\Delta t = \Delta t_0$, we have a relation similar as in quasilinear theory, namely:

$$D(\Delta t_0, J_0) = \varepsilon^2 \tau_{aco}$$

with

$$\tau_{aco} = \tau_{ac}(\Delta t_0).$$

Usually one expects that the quasilinear theory is valid if τ_{ac} is sufficiently smaller than ω_b^{-1} , where ω_b is the bounce frequency for a trajectory which is trapped by a typical resonant mode. To calculate the latter quantity, let us assume that a particular mode (m, n) is resonant for $J = J_0$, and that the interaction energy is of the following type:

$$\begin{aligned}
H_1 &= 2 |H_{mn}| \cos(\varphi + \delta), \\
\varphi &= m\theta - nt; \quad \delta = \text{const.}
\end{aligned}$$

Then it is easy to evaluate the angular velocity for small-amplitude oscillations of $J - J_0$, with the following result:

$$\omega_b = m \sqrt{|\omega'_{mn} 2 H_{mn}(J_0)|}.$$

Of course, we expect diffusion only if several modes are present, and if $|H_{mn}|$ for any mode is not smaller than the critical value according to (4); this leads to the following minimum value for the corresponding bounce frequencies:

$$\omega_b \geq \omega_{b \min} \equiv \frac{m \Gamma}{4(m+1)} \cdot \text{Min}(|\omega_{mn}|, |1 - \omega_{mn}|).$$

The true local bounce frequency is then

$$\omega_b = |H_{mn}/H_{mn \text{ crit}}|^{1/2} \omega_{b \min}.$$

The condition $\tau_{\text{aco}}\omega_b \ll 1$ is less and less fulfilled if the amplitudes $|H_{mn}|$ increase; but a necessary condition that a quasilinear description is possible at all is given as follows:

$$\tau_{\text{aco}}\omega_b \min \ll 1 .$$

It is remarkable that this condition is independent from a rescaling of the amplitudes; it depends only on the resonant frequencies $|\omega_{mn}|$ of the equilibrium, the stochasticity parameter Γ , and the shape of the spectrum of H_1 .

3. Two Examples

a) Acceleration of Particles by Random Waves

Let L be the periodicity length in space (one dimension only), and T the basic time period of the waves; then we may write the phase of a partial wave (m, n) as follows:

$$m\theta - nt = k_m \xi - \omega_n \tau ,$$

with

$$k_m = \frac{2\pi}{L} m ; \quad \omega_n = \frac{2\pi}{T} n ,$$

$$\xi = L \frac{\theta}{2\pi} ; \quad \tau = T \frac{t}{2\pi} .$$

Here, ξ is the position of the particle at the physical time τ ; its velocity is, therefore,

$$v = \frac{d\xi}{d\tau} = \frac{L}{T} \frac{d\theta}{dt} = \frac{L}{T} \frac{\partial H}{\partial J} .$$

Since the interaction energy depends on ξ and τ only we have

$$\frac{\partial H}{\partial J} = \frac{dH_0(J)}{dJ} \equiv \omega(J) ,$$

and, therefore,

$$v = (L/T)\omega(J) .$$

On the other hand, we know the following relation which must hold identically in J :

$$H_0(J) = \int_0^J \omega(J') dJ' \sim v^2 \sim \omega^2(J) .$$

Therefore, $\omega(J)$ is a linear function with constant shear parameter α :

$$\omega(J) = \alpha J .$$

The equation of motion is then as follows:

$$\frac{dv}{d\tau} = \frac{2\pi\alpha L}{T^2} \frac{dJ}{dt} = -\alpha(L/T)^2 \frac{\partial H_1}{\partial \xi} \equiv -\frac{\partial \Phi}{\partial \xi} .$$

The relevant acceleration potential is obviously

$$\Phi = \alpha(L/T)^2 H_1 .$$

For a particle with unit mass and unit charge this is also the interaction energy, so we may put

$$\alpha(L/T)^2 = 1 ,$$

and the Fourier mode of the critical potential is then given by (4), namely:

$$2|\Phi_{mn}|_{\text{crit}} = \left[\frac{\Gamma}{4} \cdot \frac{k_1}{k_m + k_1} \right]^2 \cdot \text{Min}(v_{mn}^2, ((L/T) - v_{mn})^2)$$

with

$$v_{mn} = \omega_n/k_m .$$

The condition (3) for $\omega(J)$ means simply that (L/T) is the highest velocity of the particle which we want to represent in its phase space. Of course, this limit should be much larger than the typical phase velocities v_{mn} of the waves, therefore, we may apply the simplification according to (5), and we find:

$$2|\Phi_{mn}|_{\text{crit}} = \frac{1}{L^2} \left[\frac{\pi}{2} \frac{\Gamma\omega_n}{k_m^2} \right]^2 , \quad (12)$$

where m has here been assumed large compared to 1. For an infinite system we have

$$|\Phi_{mn}| \sim L^{-1} \rightarrow 0 ,$$

but (12) asserts that $|\Phi_{mn}|_{\text{crit}}$ goes faster to zero, indicating that the stochasticity condition is trivially satisfied, and we find the usual quasilinear formulae for the diffusion coefficient and the autocorrelation time (see appendix). But for a finite system (12) is nontrivial; it predicts stochastic acceleration (or deceleration) of a particle with velocity v only if there are resonant waves with an amplitude of at least $(\pi\Gamma/2k_m L)^2$ times the kinetic energy of the particle. Let us assume, e.g., an ensemble of plasma waves with $\omega_n \approx \omega_{pe} = \text{const}$, and with the property

$$|\Phi_{mn}| \geq |\Phi_{mn}|_{\text{crit}} \quad \text{for} \quad k_{m1} \leq k_m \leq k_{m2} .$$

Then one would expect chaotic particle orbits in the interval

$$\frac{\omega_{pe}}{k_{m2}} \leq v \leq \frac{\omega_{pe}}{k_{m1}},$$

and no “heating” outside this interval. Of course, the reasoning with overlap of resonances is only qualitative – we used only Γ instead of a definite number –, and the heating process may be different from ordinary quasilinear diffusion.

b) Tracing of Toroidal Magnetic Field Lines

Here θ is an angle along the short way around a toroidal magnetic surface, and t is the angle for the long way; therefore, the periodicity interval of 2π is appropriate in both cases. The action variable J labels the magnetic surfaces and is proportional to the toroidal magnetic flux inside the torus. The stochastic stability of magnetic surfaces has recently been studied using the following model for the equilibrium and the fluctuations [15]:

$$\omega(J) = (1 + 5J^2)^{-1}; \quad 0 \leq J \leq 1, \\ H_1 = \sum_{m=3}^{11} \mathcal{C}_m \cos(m\theta - 2t); \quad \mathcal{C}_m = \frac{\varepsilon'}{(m+1)^2}, \quad (13)$$

where ε' is an adjustable parameter. The rotation number $\omega(J)$ (inverse safety factor) of the equilibrium field equals 1 at the magnetic axis ($J = 0$) and drops outwards, corresponding to the typical current profiles in tokamaks. The interaction “energy” H_1 is the perturbation of the poloidal flux function; it has been chosen by this manner because all modes $m = 3, 4, \dots, 11$, are resonant within the unit interval of J , with increasing values of J_{mn} . The coefficients \mathcal{C}_m resemble the critical Fourier modes of (4); they don’t match them exactly because the shear factor $|\omega'_{mn}|$ becomes larger than ω_{mn}^2 with increasing m , i.e. increasing J_{mn} . For our model we have

$$\omega_{mn}^2 / |\omega'_{mn}| = 1 / (10 J_{mn}),$$

and we expect that with increasing ε' the border of stable local KAM surfaces (“islands”) moves from large to small m , i.e. from the outer resonances to the inner ones. This has also been observed numerically, and the last island ($m = 3$) was destroyed for $\varepsilon' \approx 0.06$, corresponding to $\Gamma \approx \sqrt{3}$. It is easily seen that our general Hamiltonian problem of

Sect. 2 can be identified with the present one by choosing

$$2H_{mn} = \begin{cases} 0 & \text{for sign}(m) \neq \text{sign}(n) \quad \text{or} \quad n \neq \pm 2 \\ \mathcal{C}_{|m|} & \text{otherwise} \end{cases} \quad (14)$$

for the appropriate values of m .

In the following section we study the time evolution of an ensemble of trajectories starting with random initial phases θ_0 of the “particles” instead of the waves. But for weak fields the difference is negligible, as can be seen from (6); the coefficients c_{mn} there have now the following properties if H_{mn} is deterministic and if θ_0 is equally distributed in the interval $[0, 2\pi]$:

$$\langle c_{mn} c_{pq}^* \rangle = m p H_{mn} H_{pq}^* \langle e^{i(m-p)\theta_0} \rangle.$$

The last factor gives zero unless $m = p$, and from (14) we conclude then that in the latter case also $n = q$ holds. Thus we have the same statistical properties as in the case of random phases of the waves. A quasilinear description of the present example would result in the following diffusion equation:

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial J} D(J) \frac{\partial}{\partial J} f,$$

where $f(J, t)dJ$ is the probability of finding a trajectory at time t in the interval dJ around J , and $D(J)$ is obtained from (A1). Let us translate $D(J)$ back into the discrete case, using an argument $J = J_m$ where the mode m is resonant:

$$D(J_m) \equiv D_m \equiv (\pi/2)(m \mathcal{C}_m)^2. \quad (15)$$

The corresponding autocorrelation time τ_m is then defined by D_m/ε^2 , where

$$\varepsilon^2 = \frac{1}{2} \sum_{m=3}^{11} (m \mathcal{C}_m)^2 = 2.475 \times 10^{-4} \quad \text{for } \varepsilon' = 0.06.$$

In the critical case of $\varepsilon' = 0.06$ we obtain then, e.g.:

$$D_m = \begin{cases} 2.0 \times 10^{-4} & \text{for } m = 3, \\ 0.85 \times 10^{-4} & \text{for } m = 6, \end{cases}$$

and

$$\tau_m = \begin{cases} 0.80 & \text{for } m = 3, \\ 0.34 & \text{for } m = 6. \end{cases}$$

Accidentally, the resonant contribution to

$D(\Delta t, J_0)$ according to (8) is exactly the same expression like D_m in (15) if we put $\Delta t = 2\pi$.

4. Numerical Results

We have performed several runs of a numerical program for the example described in Sect. 3 b, varying ε' and J_0 , and controlling the numerical accuracy. The latter task was possible (in contrast to [15]) because we considered only the initial time evolution of the ensemble. From observation of the ensemble averages $\langle J \rangle$ and $\langle J^2 \rangle$ as functions of time we determined the beginning of the Taylor series of $D(J)$ with respect to $(J - J_0)$, starting near several resonant values of J (e.g. $J_0 = 0.316$ for $m = 3$; $J_0 = 0.65$ for $m = 6$, etc.). The procedure is roughly as follows: From the quasilinear diffusion equation one finds

$$\frac{d}{dt} \langle J \rangle = \langle \partial D(J) / \partial J \rangle, \quad (16a)$$

$$\frac{d}{dt} \langle J^2 \rangle = 2 \langle \partial [JD(J)] / \partial J \rangle. \quad (16b)$$

Here we can insert for $D(J)$, e.g. a linear relation with two unknown coefficients D_0 and a :

$$D(J) = D_0 + a(J - J_0).$$

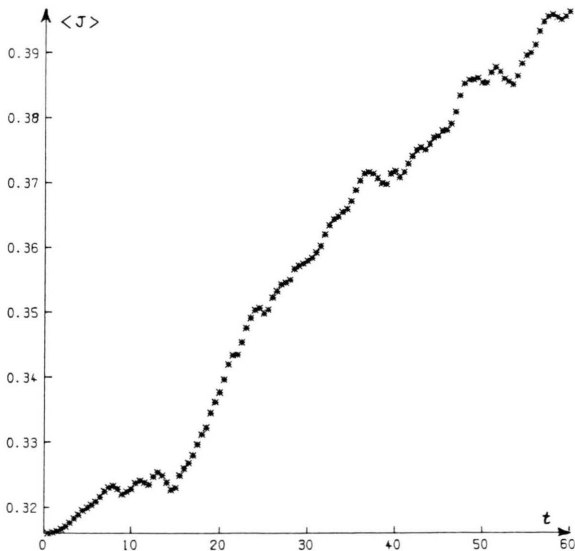


Fig. 1. Ensemble average $\langle J \rangle$ of the action variable J as function of time for 100 trajectories, starting at the marginally unstable resonance $m = 3$ with random phases.

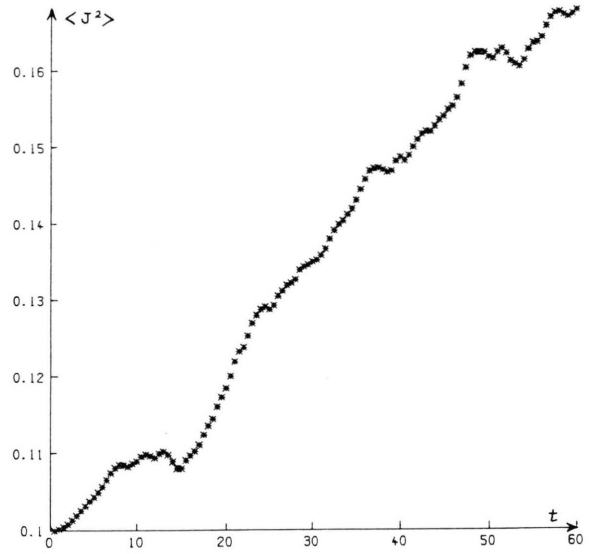


Fig. 2. $\langle J^2 \rangle$ as function of time for the same run as in Figure 1.

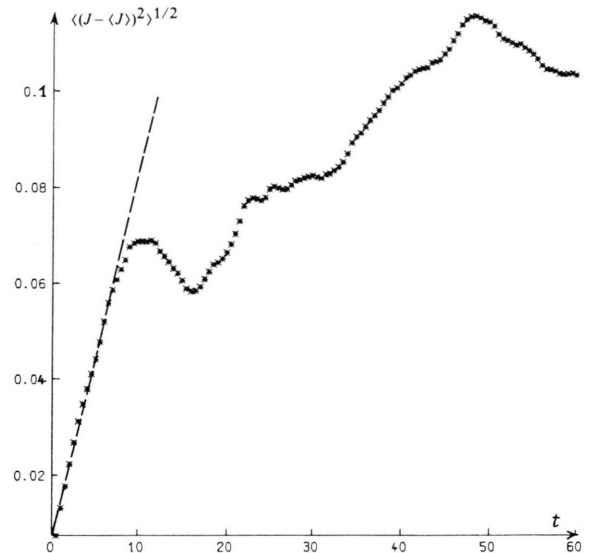


Fig. 3. Root-mean-square of $J - \langle J \rangle$ as obtained from Figs. 1 and 2 as function of time.

These coefficients are then determined from the mean initial slopes of $\langle J \rangle$ and $\langle J^2 \rangle$. Of course, the evolution could be non-diffusive at all, therefore, we observed also the variance $\langle (J - \langle J \rangle)^2 \rangle$ or the square root of it. The exact details and the main part of the numerical material will be given elsewhere [19]. Here we show only two examples for $\varepsilon' = 0.06$ where the mode $m = 3$ is just at its

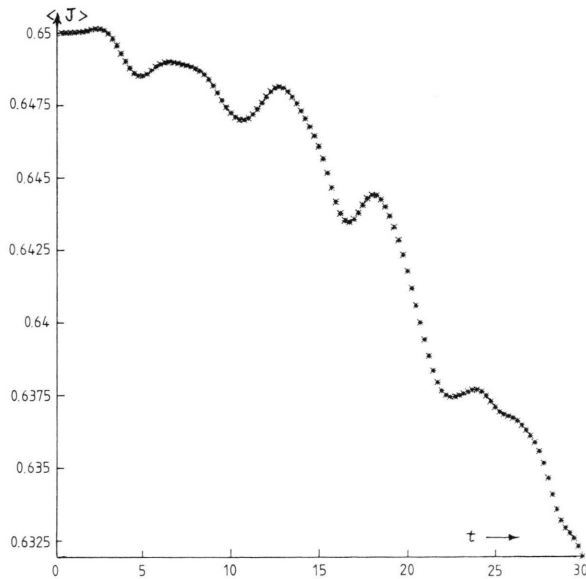


Fig. 4. Time evolution of $\langle J \rangle$ for 250 trajectories starting at the more unstable resonance $m = 6$ with random phases.

threshold of stochasticity, while the amplitude of the mode $m = 6$ is by a factor 2 above its threshold value; but the main features and conclusions may already be obtained here.

From the Figs. 1 and 2 where we started at the marginally unstable resonance $m = 3$ we obtain within the interval $0 \leq t \leq 10$:

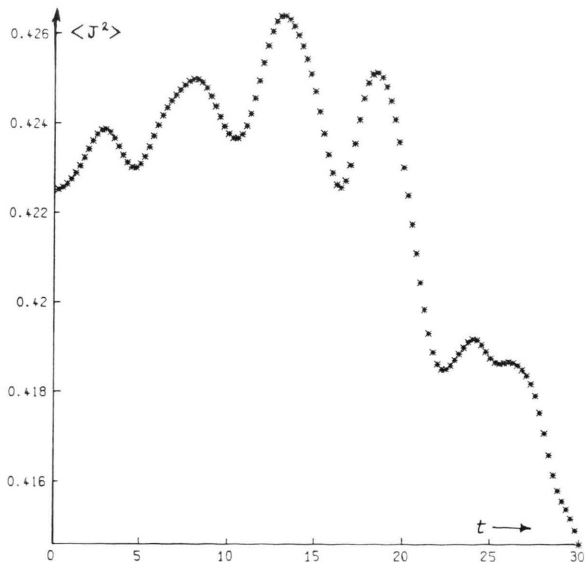


Fig. 5. Time evolution of $\langle J^2 \rangle$ for the same run as in Figure 4.

$$D_0 = 2.3 \times 10^{-4}; \quad a = 7.7 \times 10^{-4} \quad (J_0 = 0.316) .$$

But Fig. 3 shows that the square root of the variance is proportional t , indicating that no diffusion takes place. At a later time we find again a linear increase but with a smaller slope. Similarly we obtain from the Figs. 4 and 5 the parameters for an ensemble of trajectories starting at the more unstable resonance $m = 6$:

$$D_0 = 2.46 \times 10^{-4}; \quad a = -1.95 \times 10^{-4} \quad (J_0 = 0.65) .$$

Here we find that the variance itself is proportional to t (Fig. 6), showing the diffusive nature of this mode.

Next we consider $D(\Delta t, J_0)$ according to (8) for both cases as function of Δt . In the first case ($J_0 = 0.316$) we find that the expression is dominated by the resonant contribution ($m = 3$) in a large interval ($0 \leq \Delta t \leq 90$), namely:

$$D(\Delta t, J_0) \approx D_3 \Delta t / 2\pi \quad (J_0 = 0.316) ,$$

where D_3 can be taken from (15) with $m = 3$. Matching with the quasilinear value leads obviously to the condition

$$\Delta t = 2\pi , \quad (17)$$

which is, however, in this case purely artificial, due to the absence of diffusion. The picture changes completely in the second case; Fig. 7 shows

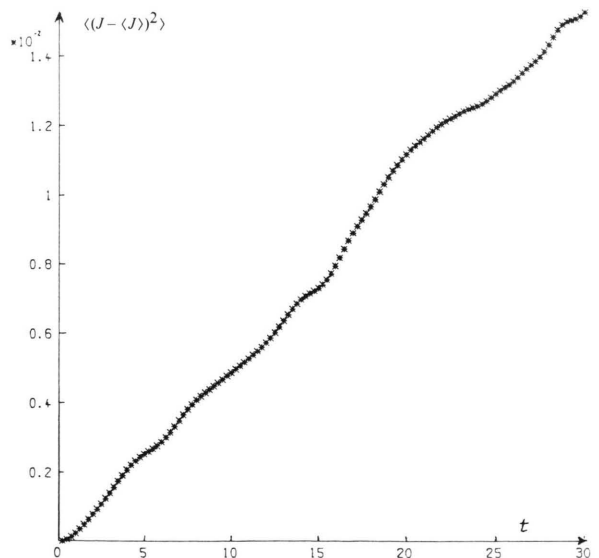


Fig. 6. Mean square of $J - \langle J \rangle$ as obtained from Figs. 4 and 5 as function of time.

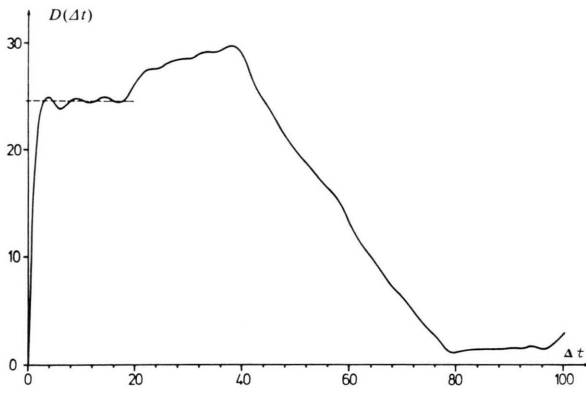


Fig. 7. The diffusion coefficient according to (8) for $J_0 = 0.65$ ($m = 6$) as function of Δt .

$D(\Delta t, J_0)$ for $J_0 = 0.65$. We find approximately a plateau in the interval

$$4 \leq \Delta t \leq 20 ,$$

consistent with (17). This confirms the diffusive nature of the mode during the initial time. It should be noted, however, that for other modes $m \neq 3$ the plateau is not so well pronounced, and no firm statements for later times or high amplitudes are possible so far.

Finally we show $D(\Delta t, J_0)$ for $\Delta t = 2\pi$ as function of J_0 (Fig. 8). The parameters (D_0, a) for three resonances ($m = 3, 4, 6$) are shown as absolute values and slopes of the curve, respectively, with

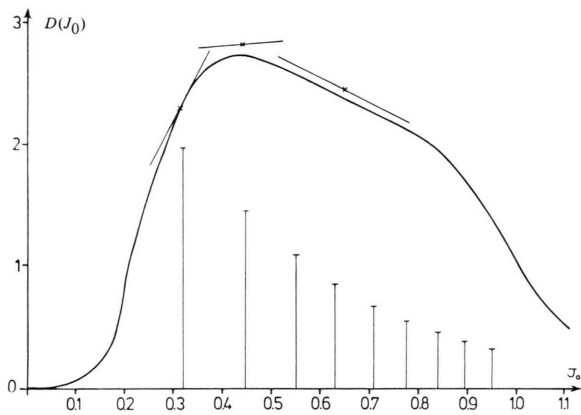


Fig. 8. The diffusion coefficient according to (8) for $\Delta t = 2\pi$ as function of J_0 ; for three values of J_0 the fit of D_0 and a from the time-evolution of the ensemble is shown. For all nine resonances we show also the contribution of the resonant mode to D .

satisfactory agreement. The figure shows also the resonant contribution to $D(\Delta t, J_0)$ for the appropriate values of J_0 ; the agreement with D is only good for the mode $m = 3$ with the largest amplitude; in all other cases the contributions of the non-resonant modes are appreciable. This explains why the true autocorrelation time $D(\Delta t, J_0)/\varepsilon^2$ is larger than the corresponding quasilinear expression, D_m/ε^2 ; nine modes and the period $L = 2\pi$ are obviously a poor representation of the thermodynamic limit.

It is also interesting to compare the autocorrelation times D_0/ε^2 and the reciprocal bounce frequencies ω_b^{-1} as explained in Sect. 2; we find

$$D_0/\varepsilon^2 = \begin{cases} 0.9 & \text{for } J_0 = 0.316 , \\ 1.0 & \text{for } J_0 = 0.65 ; \end{cases}$$

$$\omega_b^{-1} = \begin{cases} 4.7 & \text{for } J_0 = 0.316 , \\ 6.2 & \text{for } J_0 = 0.65 . \end{cases}$$

Even the marginally stochastic mode $m = 3$ fulfills the condition $\tau_{ac}\omega_b < 1$, and Fig. 9 shows that it also becomes diffusive at later times, but with a smaller diffusion coefficient than given implicitly by (8); to evaluate (8) (which is a Lagrangian dif-

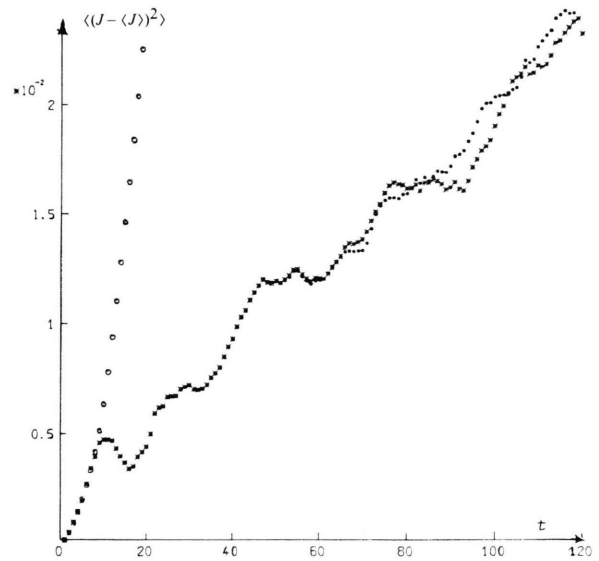


Fig. 9. Mean square of $J - \langle J \rangle$ for the same trajectories as in Figs. 1–3, but for a longer time. Crosses: The same maximal integration error of 10^{-3} per time step as in Figs. 1–3. Dots: maximal integration error of 10^{-6} per time step. Circles: Prediction of (18).

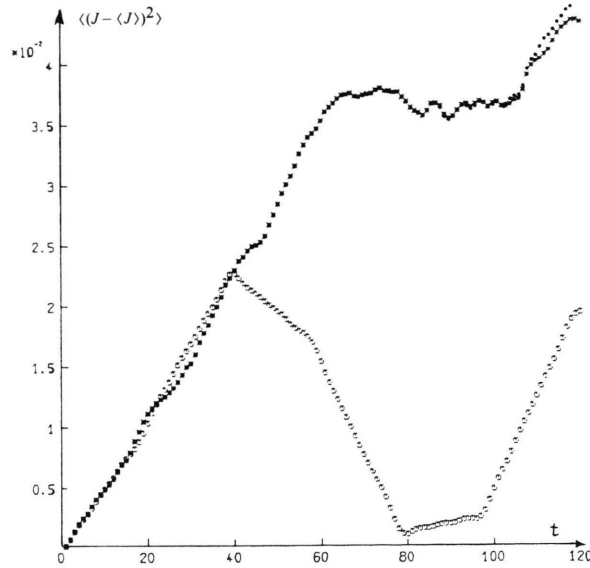


Fig. 10. The same as Fig. 9, but for the trajectories described in Figures. 4–6.

fusion coefficient), we can use the following identity:

$$\langle (J - \langle J \rangle)^2 \rangle = 2tD(t, J_0) - (\langle J \rangle - J_0)^2. \quad (18)$$

The circles in Fig. 9 show the right-hand side of (18); obviously one has to evaluate a time-dependent diffusion equation to match the real evolution for $t > 10$. Figure 10 shows that the evolution of the trajectory with $J_0 = 0.65$ is well represented up to $t = 40$. Then again we find that the theoretical description has to be refined; in particular it has to show the saturation effect at $t \approx 70$ which is a real phenomenon, not due to the numerical instability. A similar effect for larger amplitudes has also been observed in [4]; it will again be discussed in [19].

5. Conclusions

We have discussed the general Hamiltonian problem in action/angle variables of a particle exposed to a discrete set of waves in one space dimension. This picture applies not only to particle acceleration, but also to the question how magnetic field lines diffuse if a symmetric magnetic field is perturbed by fluctuations. First we derived perturbatively expressions for the (Lagrangian) diffusion coefficient and autocorrelation time for an ensemble of waves with random phases at $t = 0$;

since we did not use the thermodynamic limit, the results depend on time. Then we calculated numerically the time evolution of some moments of the action variable according to a previously studied model for magnetic field lines on a torus [15]. If the trajectories start from a point in phase space where the overlap condition is just marginally satisfied, we find a short phase of free acceleration, then a long phase of diffusion; only the first phase can be fitted to the perturbative treatment. If the trajectories start from a level of twice the stochasticity threshold, we observe diffusive behaviour from the beginning; it is initially well represented by the perturbative treatment if the contribution of non-resonant modes is included. However, at later times where the theoretical formula fails we find a saturation of the diffusion; its origin is not a numerical effect, but it is not yet understood. A similar effect at larger amplitudes has also been observed in [4]. The best way to analyze and to represent the problem is in terms of cumulants because these turn out to be relatively smooth functions of time – though we used only nine individual modes and 100 or 250 members of the ensemble to represent the spectrum. However, the comparison with any theory requires also the time integration of the corresponding kinetic equations; the simple perturbative formulas fail long before the numerical accuracy is lost.

It might be interesting to combine our analysis valid on a short time scale with the approach of Mackay et al. [13, 22]. They assume the trajectories to move from one cantorus to another in a single toroidal cycle and calculate probabilities for crossing these partial barriers. Then it is possible to compute the average number of toroidal cycles needed to cross all resonances in terms of Markov-chains. Their results could most probably be improved by taking into account that a trajectory migrates more or less slowly between the cantori; in doing so, the mean duration of stay between the barriers may be estimated using the analytically calculated diffusion coefficient.

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Appendix

Here we apply the thermodynamic limit to the first of the examples in Sect. 3, the stochastic particle acceleration problem. The equation of motion considered there is

$$\frac{dv}{d\tau} = -\frac{\partial}{\partial \xi} \Phi ,$$

where Φ is the potential energy for a particle with unit mass and charge. Starting with the Fourier representation for Φ in a system of finite length L we want to keep constant the mean energy density of the electric field for $L \rightarrow \infty$ and $T \rightarrow \infty$; this gives

$$\langle (\partial \Phi / \partial \xi)^2 \rangle = \sum_{m,n} |k_m \Phi_{mn}|^2 \rightarrow \int dk \int d\omega k^2 \mathcal{J}(k, \omega) < \infty ,$$

where $\mathcal{J}(k, \omega)$ is the (smooth, localized, non-negative) spectral function for the infinite system. Here we used again the approximations of Sect. 2 (unperturbed orbits, random phases at $t = 0$). We have also

$$\sum_{m,n} \simeq \frac{L \cdot T}{(2\pi)^2} \int dk \int d\omega ; \quad k_m \simeq k ,$$

so we find

$$|\Phi_{mn}| \simeq \frac{2\pi}{\sqrt{L \cdot T}} [\mathcal{J}(k, \omega)]^{1/2} .$$

Since the time interval Δt of Sect. 2 was a definite fraction or multiple of the “time” period 2π of t we keep it fixed in the limit $T \rightarrow \infty$; therefore, the corresponding physical time interval $\Delta \tau$ goes to infinity:

$$\Delta \tau = T(\Delta t / 2\pi) \rightarrow \infty .$$

With the further relations of Sect. 3 a) we have

$$\frac{\langle (\Delta v)^2 \rangle}{2 \Delta \tau} = (\alpha L / T)^2 \frac{\langle (\Delta J)^2 \rangle}{2 \Delta t} \cdot \frac{2\pi}{T} ,$$

and the quasilinear diffusion coefficient D_{QL} is then obtained from the corresponding expression (8) as follows (since $|c_{mn}|^2 = (L/2\pi)^2 k_m^2 |\Phi_{mn}|^2$):

$$\begin{aligned} D_{QL} &= \lim_{\substack{\Delta \tau \rightarrow \infty \\ L \rightarrow \infty}} \frac{\langle (\Delta v)^2 \rangle}{2 \Delta \tau} \\ &= \lim \alpha \cdot \left(\frac{2\pi}{T} \right)^2 \cdot \sum_{m,n} (L/2\pi)^2 \frac{k_m^2 |\Phi_{mn}|^2}{(\Omega_{mn})^2 \Delta \tau} \\ &\quad \cdot [1 - \cos(\Omega_{mn} \Delta \tau)] \end{aligned}$$

with

$$\Omega_{mn} = \omega_n - k_m v \simeq \Omega ; \quad v = (L/T) \omega (J)$$

$$\text{and } \alpha (L/T)^2 = 1$$

as in Sect. 3 a). With the replacements as indicated above we obtain then:

$$D_{QL} = \lim \int dk \int d\omega \frac{k^2 \mathcal{J}(k, \omega)}{\Omega^2 \Delta \tau} 2 \sin^2[\Omega \Delta \tau / 2] .$$

Now we put

$$y = \Omega \Delta \tau / 2 ; \quad dy = d\omega (\Delta \tau / 2) ,$$

$$\omega = y(2/\Delta \tau) + kv \rightarrow kv \quad \text{for fixed } y ,$$

and the limit $\Delta \tau \rightarrow \infty$ can easily be performed; the result is

$$\int_{-\infty}^{+\infty} dy \frac{\sin^2 y}{y^2} = \int_{-\infty}^{+\infty} dy' \frac{\sin y'}{y'} = \pi , \quad \text{and}$$

$$\begin{aligned} D_{QL} &= \pi \int dk k^2 \mathcal{J}(k, \omega = kv) \\ &= \pi \int dk \int d\omega k^2 \mathcal{J}(k, \omega) \delta(\omega - kv) . \end{aligned} \quad (\text{A1})$$

This is the resonant part of the quasilinear diffusion coefficient; the non-resonant part does not appear because the particle could not react back on the waves [23]. Similarly we can calculate the Lagrangian autocorrelation time of the electric field; in (11) we have first to perform the thermodynamic limit, then its dependence on Δt again vanishes. The result enables us to write (A1) in the following form:

$$D_{QL} = \varepsilon^2 \tau_{ac} ,$$

where

$$\varepsilon^2 = \int dk \int d\omega k^2 \mathcal{J}(k, \omega) .$$

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