

Diffusion in Phase Space

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1. Introduction.

In order to study diffusion in any region of phase space containing nested closed curves we choose action-angle variables, γ, J . The action J labels each closed phase curve and is equal to its area divided by 2π . We can introduce rectangular variables Q, P by the equations

$$\begin{aligned} Q &= (2J)^{1/2} \sin \gamma, \\ P &= (2J)^{1/2} \cos \gamma, \end{aligned} \tag{1.1}$$

where the angle variable γ is measured clockwise from the P -axis. The phase curves are circles in the Q, P plane with radius $(2J)^{1/2}$. We assume that the motion consists of a Hamiltonian motion along a curve of fixed J (in the original coordinate system and in the system Q, P) plus a diffusion and a damping which can change the value of J .

Now consider a system of particles described by a density $\rho(J, t)$, so that the number of particles between the curves J and $J+dJ$ is

$$dN = \rho(J, t) dJ. \tag{1.2}$$

These cN particles are distributed uniformly in the phase space between the curves J and $J+dJ$.

2. The Diffusion Equation.

Let $I(J)$ be the net current of particles per second passing any orbit J , defined as positive in the direction of increasing J . I is a sum of a diffusion current and a damping current:

$$I(J, t) = -D(J) \frac{\partial \rho}{\partial J} - \frac{\rho J}{2\tau}. \tag{2.1}$$

The diffusion current is by definition proportional to $-\partial \rho / \partial J$ with a diffusion constant $D(J)$ which may depend on J . The damping current is negative and is proportional to ρ and inversely proportional to the damping time τ ; we will show in a moment that it also contains the factor $J/2$.

The time rate of change of the number of particles in the interval dJ is

$$\frac{\partial \rho}{\partial t} dJ = I(J) - I(J + dJ) = -\frac{\partial I}{\partial J} dJ . \quad (2.2)$$

We substitute from Eq.(2.1) to obtain the diffusion equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial J} \left(D(J) \frac{\partial \rho}{\partial J} \right) + \frac{\partial}{\partial J} \left(\frac{\rho J}{2\tau} \right) . \quad (2.3)$$

This is a continuity equation for the particle density ρ . It guarantees that particles are conserved in the region where it holds, though they may flow in or out at the boundaries.

If we put $D(J) = 0$, the general solution of Eq.(2.3) is

$$\rho(J,t) = e^{t/2\tau} F(Je^{t/2\tau}) , \quad (2.4)$$

as may be verified by direct substitution, where $F(w)$ is an arbitrary function. Equation (2.4) is what we want, since it says that $\rho(J,t)dJ$ remains constant if the J of each particle damps with the time constant 2τ , where τ is the time constant for the damping of the amplitude $(2J)^{1/2}$.

Equation (2.3) requires two boundary conditions and the initial function $\rho(J, 0)$. One boundary condition is that the current (2.1) must vanish at the origin $J=0$. The second is often that the density $\rho(J_b, t)$ vanish at a boundary value J_b , which may for example be the curve that intersects the vacuum chamber wall, or a separatrix beyond which the motion quickly becomes unbounded.

3. The Diffusion Coefficient.

To find the diffusion coefficient from first principles, we would need to study the changes in J produced by whatever collisions and other processes are causing the diffusion. At this point we will avoid this problem by using the fact that we know the effect of diffusion and damping in an infinite aperture is to produce a Gaussian equilibrium distribution in the amplitude $(2J)^{1/2}$:

$$\rho(J,\infty) = N \frac{e^{-J/\sigma^2}}{\sigma^2} , \quad (3.1)$$

where σ is the rms emittance of the equilibrium beam and N is the total number of particles. Note that the details of the scattering processes which cause the diffusion are now buried in the constant σ .

At equilibrium $\rho(J)$ does not depend on t , so Eq.(2.3) requires that the current be constant:

$$-D(J)\frac{\partial\rho}{\partial J} - \frac{J\rho}{2\tau} = \text{constant} = 0, \quad (3.2)$$

where we use the boundary condition that the current must vanish at $J=0$. We substitute from Eq.(3.1) to obtain the diffusion coefficient:

$$D(J) = \frac{J\sigma^2}{2\tau}. \quad (3.3)$$

Note that this form of the diffusion coefficient guarantees that the current (2.1) will vanish at $J = 0$, provided the density $\rho(J)$ is well-behaved there. Equation (2.3) has a singular point at $J = 0$, with the diffusion constant (3.3). We will see in the next section that near $J = 0$, there are both well-behaved and ill-behaved solutions of Eq.(2.3). The boundary condition then selects the well-behaved solution there.

4. Diffusion to a Boundary.

We now consider diffusion from a region in phase space bounded by a boundary J_b and solve Eq.(2.3) in the region $0 \leq J \leq J_b$. Let us solve Eq.(2.3) by expanding $\rho(J, t)$ in eigenfunctions of the operator on the right side of Eq.(2.3):

$$\rho(J, t) = \sum_{\ell} c_{\ell} \rho_{\ell}(J) e^{-\frac{t}{\tau_{\ell}}}, \quad (4.1)$$

where $\rho_{\ell}(J)$, τ_{ℓ} satisfy the eigenvalue equation

$$\frac{\partial}{\partial J} \left(\frac{\sigma^2 J}{2\tau} \frac{\partial \rho_{\ell}}{\partial J} \right) + \frac{\partial}{\partial J} \left(\frac{J \rho_{\ell}}{2\tau} \right) = -\frac{1}{\tau_{\ell}} \rho_{\ell}, \quad (4.2)$$

and the constants c_{ℓ} are chosen to satisfy the initial condition. One boundary condition requires that the eigenfunctions vanish at $J = J_b$. At $J = 0$ the current will necessarily vanish unless $\partial \rho_{\ell} / \partial J$ is infinite. If we substitute for $\rho(J)$ in Eq.(4.2) a power series whose first term goes like J^r , we find in the standard way that $r^2 = 0$, so that there is a double root at $r = 0$, and we have only one solution (apart from an arbitrary constant factor). This is the well-behaved solu-

tion picked out by the boundary condition at the origin. The other solution turns out to behave like $\ln(J)$ near the origin.

On physical grounds, we expect the eigenvalues $(-1/\tau_\ell)$ to be negative, so that the solutions are damped with time constants τ_ℓ . If we arrange the eigenvalues τ_0, τ_1, \dots in increasing order, then after some time the solution (4.1) will be approximated by its first term and will damp exponentially with time constant τ_0 , keeping its characteristic shape $\rho_0(J)$, provided that the next smallest time constant τ_1 is not too close to τ_0 . The solution consists of an initial transient described by the remaining terms in the sum plus a final state whose shape is independent of the initial distribution.

Note that for an infinite aperture the smallest eigenvalue of Eq.(4.1) is zero (τ_0 is infinite) and the corresponding normalized eigenfunction is the solution (3.1) with $N=1$. The general solution will again contain an initial transient depending on the initial distribution.

We can convert Eq.(4.2) to an integral equation. Equation (4.2) can be integrated immediately to obtain

$$\frac{\partial \rho_\ell}{\partial J} + \frac{\rho_\ell}{\sigma^2} = -\frac{2\tau}{\sigma^2 \tau_\ell} \int_0^J \rho_\ell dJ, \quad (4.3)$$

where we have applied the boundary condition that the current vanishes at $J=0$. The left side has the integrating factor e^{J/σ^2} . We multiply by this factor and integrate again:

$$\rho_\ell(J) = \rho_\ell(0)e^{-J/\sigma^2} - \frac{2\tau e^{-J/\sigma^2}}{\sigma^2 \tau_\ell} \int_0^J \frac{e^{J'/\sigma^2}}{J'} \left(\int_0^{J'} \rho_\ell dJ' \right) dJ. \quad (4.4)$$

This is the integral equation for the eigenfunction ρ_ℓ . Note that if we solve the equation iteratively by repeatedly substituting the right hand side for ρ_ℓ in the integral, we obtain ρ_ℓ as a power series in τ_ℓ^{-1} . If after N iterations we use the result to apply the boundary condition at $J = J_b$, we can solve for the N largest values of τ_ℓ .

The first term in the solution (4.4) is the steady state solution (3.1) corresponding to an infinite τ_ℓ . Let us normalize it (approximately) to correspond to one particle:

$$\rho_\ell(J) = \frac{e^{-J/\sigma^2}}{\sigma^2}, \quad (\text{zeroth approximation}). \quad (4.5)$$

This normalization does not quite correspond to a single particle both because it is to be integrated only to $J = J_\ell$ and because it is only the first term in a series. If we substitute this into the integral in Eq.(4.4) we get the second term in the series. The inner integral can be evaluated immediately:

$$\rho_\ell(J) = \frac{e^{-J/\sigma^2}}{\sigma^2} - \frac{2\tau e^{-J/\sigma^2}}{\sigma^2 \tau_\ell} \int_0^{J/\sigma^2} \frac{e^w - 1}{w} dw, \quad (\text{first approximation}). \quad (4.6)$$

This could be substituted into the integral in Eq.(4.4) to get a second approximation, and so on. If $J \gg \sigma^2$, then the first approximation (4.6) should be a good approximation to the eigenfunction ρ_0 corresponding to the smallest eigenvalue τ_0^{-1} .

If we apply the boundary condition $\rho_0(J_b) = 0$ to the first approximation (4.6), we can solve for τ_0 :

$$\tau_0 = 2\tau \int_0^\xi \frac{e^w - 1}{w} dw = 2\tau [\text{Ei}(\xi) - \ln \xi - \gamma], \quad (\xi \gg 1), \quad (4.7)$$

where

$$\xi = \frac{J}{\sigma^2}. \quad (4.8)$$

Equation (4.7) involves an exponential integral. Since it is only valid when $\xi \gg 1$, we can evaluate it as follows:

$$\begin{aligned} \int_0^\xi \frac{e^w - 1}{w} dw &= \int_0^2 \frac{e^w - 1}{w} dw - \int_2^\xi \frac{dw}{w} + \int_2^\xi \frac{e^w}{w} dw \\ &= C_2 - \ln \frac{\xi}{2} + \frac{e^\xi}{\xi} \left[1 + \frac{1}{\xi} + \frac{2}{\xi^2} + \dots \right] \\ &\rightarrow \frac{e^\xi}{\xi} \end{aligned} \quad (4.9)$$

where the constant C_2 includes the first integral and the contribution from the lower limit of the third. We have chosen to break the integral at $J=2$ so that successive terms in the bracket in the second line will grow smaller; any number greater than 1 would do. The last term in the second line is obtained by successive integrations by parts. In the last line we have written only the

dominant term for large ξ . If we substitute in Eq.(4.7) we obtain the Sands formula:

$$\tau_0 = 2\tau \frac{e^{\xi}}{\xi} . \quad (4.10)$$

Note that this derivation requires no enquiry into the details of the scattering process causing the diffusion nor the process causing the damping. The formula applies to diffusion caused by quantum emission, gas scattering, or any other multiple scattering processes; we need only know the damping time and the net rms width σ of the resulting gaussian distribution for an infinite aperture.

In the form (4.7) our formula approaches zero as it should for $\xi=0$:

$$\tau_0 = 2\tau \left[\xi + \frac{\xi^2}{4} + \dots \right] , \quad (4.11)$$

although this formula is not accurate since formula (4.7) holds only for large values of ξ .

5. Some Technical Questions.

It is not clear that Eq.(4.1) represents the general solution of Eq.(2.3) The operator in the left member of Eq.(4.2) is not self-adjoint, so its eigenfunctions may not in general be orthogonal, nor do they necessarily form a complete set.

However the solution for the largest eigenvalue τ_0 does correspond to an exponentially decaying solution which should remain after initial transients have disappeared. If we can solve for the next highest eigenvalue τ_1 , that will give an indication of the time required for the transients to die out.

Let us find the second eigenvalue for the problem discussed in Section 4 above. To simplify the algebra, let us replace the action variable J by the dimensionless variable

$$w = J / \sigma^2 , \quad (5.1)$$

and renormalize ρ_l to the integration variable w . Eq.(4.4) then becomes

$$\rho_l(w) = e^{-w} - \frac{2\tau}{\tau_l} e^{-w} \int_0^w dw' \frac{e^{w'}}{w'} \int_0^{w'} \rho_l(w'') dw'' . \quad (5.2)$$

The first approximation (4.6) to the solution is

$$\rho_\ell(w) = e^{-w} - \frac{2\tau}{\tau_\ell} e^{-w} \int_0^w \frac{e^{w'} - 1}{w'} dw' \approx e^{-w} - \frac{2\tau}{\tau_\ell w}, w \gg 1. \quad (5.3)$$

We need only the asymptotic value of ρ_ℓ for large w . We substitute this into Eq.(5.2) to obtain the second approximation:

$$\begin{aligned} \rho_\ell(w) &\approx e^{-w} - \frac{2\tau}{\tau_\ell w} + \frac{2\tau e^{-w}}{\tau_\ell} \int_0^w dw' \frac{e^{w'}}{w'} \int_0^{w'} \frac{2\tau dw''}{\tau_\ell w''} \\ &\approx e^{-w} - \frac{2\tau}{\tau_\ell w} + \left(\frac{2\tau}{\tau_\ell} \right)^2 \frac{\ln w}{w}, \end{aligned} \quad (5.4)$$

where we have kept only the dominant terms for large w . We now apply the boundary condition:

$$\rho_\ell(\xi) = 0 = e^{-\xi} - \left(\frac{2\tau}{\tau_\ell} \right) \frac{1}{\xi} + \left(\frac{2\tau}{\tau_\ell} \right)^2 \frac{\ln \xi}{\xi}, \quad (5.5)$$

whose two roots for $\xi \gg 1$ are

$$\tau_0 = 2\tau \frac{e^\xi}{\xi}, \quad \tau_1 = 2\tau \ln \xi. \quad (5.6)$$

The first solution is the Sands formula for the final decay time. The second gives the decay time for the longest lasting part of the initial transient. Note that τ_1 becomes infinite for large ξ , but much more slowly than τ_0 , so that the transient does indeed die out rapidly compared with the final decay rate. Note also that the second eigenfunction ρ_1 has one node near $w=\xi$, but it is not orthogonal to ρ_0 ; it is nearly equal to ρ_0 over most of the range of w , so we would need higher-order eigenfunctions to match the most likely initial distributions, even assuming they are a complete set. The fact that ρ_1 differs from ρ_0 only in the tail of the distribution reflects the fact that the tail is the region which damps most slowly into the final configuration.

If we try to take the limit of an infinite aperture ($\xi \rightarrow \infty$) both decay times go to infinity, so we fail to find the transient for the infinite aperture case.

Numerical solution of Eq.(2.3) should yield the complete solution in any case.

6. Diffusion Between Islands.

Let us study the diffusion of beam between the islands and the central triangle near a third-integral resonance. We have to solve the diffusion equation (2.3) in two separate regions, the islands ($0 \leq J \leq J_{bl}$) and the central triangle ($0 \leq J \leq J_{bc}$). The solutions are linked by boundary conditions which specify the current from the islands to the center and vice versa which are proportional to the densities at the boundaries:

$$I_{I \rightarrow C} = k_I \rho(J_{bl}) \quad , \quad I_{C \rightarrow I} = k_C \rho(J_{bc}) \quad . \quad (6.1)$$

We are assuming that the damping time is short compared with the diffusion time, so that we can neglect the time spent by a particle in the outer region beyond the islands. Any particle escaping into this region will quickly damp into either the islands or the central triangle. If this were not the case, we would have to solve also for the diffusion in the outer region with equations like (6.1) connecting it with the islands and the central triangle.

We can evaluate the constants k in Eq.(6.1). We note that except near a fixed point the separatrices which bound the various regions are locally indistinguishable from any other phase curve. We recognize a separatrix only by viewing it globally. The processes, scattering and damping, which drive particles across a separatrix are local and hence the same as those which drive a particle across any phase curve. Moreover since they are local we can evaluate the current across any phase curve as if the region in which it is located extended to infinity. Let us therefore take the equilibrium case [e.g. the solution (3.1)] when the total current is zero. The current is given by Eq.(3.2) in which we have a balance between an outward diffusion and an equal inward damping. The outward diffusion current is equal and opposite to the second term, so the constants k in Eq.(6.1) are

$$k_I = \frac{\alpha_I J_{bl}}{2\tau_I} \quad , \quad k_C = \frac{\alpha_C J_{bc}}{2\tau_C} \quad , \quad (6.2)$$

where α_I is the fraction of particles diffusing out of the islands which go into the central triangle, and α_C is the corresponding fraction diffusing from the center into the islands. The constants τ are the damping times which may be different for the islands and for the central triangle. The reader who does not accept this argument may regard the constants α as suitably chosen constants which give the correct values for the constants k .

Let us first find the steady state solution. Equation (2.3) tells us, just as in Section 3, that in the steady state the currents are constant and by the

boundary condition at $J=0$ the currents must be zero. The solutions are then the same as in Eq.(3.1):

$$\rho_I(J, \infty) = N_I \frac{e^{-J/\sigma_I^2}}{\sigma_I^2} , \quad \rho_C(J, \infty) = N_C \frac{e^{-J/\sigma_C^2}}{\sigma_C^2} , \quad (6.2)$$

where N_I and N_C are approximately the number of particles in the islands and the central triangle respectively. The solutions (6.2) extend only out to the boundaries, but if $J \gg \sigma$ for both regions then the integral of $\rho(J)$ from the center to the boundary of either region will give nearly the coefficient N .

Since the net current is zero, the boundary conditions require that the two currents (6.1) be equal:

$$I_{I \rightarrow C} = k_I N_I \frac{e^{-J_{bl}/\sigma_I^2}}{\sigma_I^2} = I_{C \rightarrow I} = k_C N_C \frac{e^{-J_{bc}/\sigma_C^2}}{\sigma_C^2} . \quad (6.3)$$

We can solve for the ratio of the particle numbers:

$$\zeta = \frac{N_I}{N_C} = \frac{\alpha_C J_{bc}}{2\tau_C} \frac{2\tau_I}{\alpha_I J_{bl}} \frac{\sigma_I^2}{\sigma_C^2} \frac{e^{J_{bl}/\sigma_I^2}}{e^{J_{bc}/\sigma_C^2}} = \frac{\alpha_C \tau_{0C}}{\alpha_I \tau_{0I}} , \quad (6.4)$$

where in the third member we have introduced the times

$$\tau_{0I} = 2\tau_I \frac{e^{J_{bl}/\sigma_I^2}}{\sigma_I^2} \quad \text{and} \quad \tau_{0C} = 2\tau_C \frac{e^{J_{bc}/\sigma_C^2}}{\sigma_C^2} \quad (6.5)$$

for the diffusion of beam from the islands and from the central triangle according to the Sands formula, i.e. if all particles are lost at the boundaries. If the total number of particles is N then we can write

$$N_I = \frac{\zeta N}{1+\zeta} , \quad N_C = \frac{N}{1+\zeta} . \quad (6.6)$$

We next seek the solution which damps at the slowest finite rate. It will have to satisfy Eq.(4.2) in both regions with the same damping time τ_1 . The boundary conditions require that the current approaching the boundary from

within each region be given by Eqs.(6.1) and (6.2):

$$\begin{aligned} -\frac{J_{bl}\sigma_I^2}{2\tau_I} \frac{\partial \rho_{II}}{\partial J} \Big|_{J_{bl}} - \frac{\rho_{II}(J_{bl})J_{bl}}{2\tau_I} &= \frac{\alpha_I J_{bl}\rho_{II}(J_{bl})}{2\tau_I} - \frac{\alpha_C J_{bc}\rho_{CI}(J_{bc})}{2\tau_C} , \\ -\frac{J_{bc}\sigma_C^2}{2\tau_C} \frac{\partial \rho_{CI}}{\partial J} \Big|_{J_{bc}} - \frac{\rho_{CI}(J_{bc})J_{bc}}{2\tau_C} &= \frac{\alpha_C J_{bc}\rho_{CI}(J_{bc})}{2\tau_C} - \frac{\alpha_I J_{bl}\rho_{II}(J_{bl})}{2\tau_I} . \end{aligned} \quad (6.7)$$

Note that the sum of these two currents is zero, giving conservation of particles. Because the boundary condition at $J=0$ is the same in all regions, the solutions of Eq.(4.2) for islands and central triangle will have the same form as in the case studied in Section 4. Near the boundaries we can use the asymptotic form given by Eqs.(4.6) and (4.9):

$$\rho_{II}(J) = C_I \left(\frac{e^{-J\sigma_I^2}}{\sigma_I^2} - \frac{2\tau_I}{\tau_I J} \right) , \quad \rho_{CI}(J) = C_C \left(\frac{e^{-J\sigma_C^2}}{\sigma_C^2} - \frac{2\tau_C}{\tau_I J} \right) , \quad (6.8)$$

where C_I and C_C are arbitrary constants. We substitute into Eq.(6.7). The first terms give no current in the left members. In the right members they can be replaced by the expressions in Eqs.(6.5). The result is

$$\begin{aligned} C_I \left(1 - \frac{\sigma_I^2}{J_{bl}} \right) \frac{1}{\tau_I} &= C_I \alpha_I \left(\frac{1}{\tau_{I0}} - \frac{1}{\tau_I} \right) - C_C \alpha_C \left(\frac{1}{\tau_{C0}} - \frac{1}{\tau_I} \right) , \\ C_C \left(1 - \frac{\sigma_C^2}{J_{bc}} \right) \frac{1}{\tau_I} &= C_C \alpha_C \left(\frac{1}{\tau_{C0}} - \frac{1}{\tau_I} \right) - C_I \alpha_I \left(\frac{1}{\tau_{I0}} - \frac{1}{\tau_I} \right) . \end{aligned} \quad (6.9)$$

The second terms in the brackets in the left members are negligible by assumption. Since the right members are equal and opposite in sign, so must be the constants C_I and C_C :

$$C_I = -C_C = 1 , \quad (6.10)$$

where we have normalized the eigenfunction ρ_I by setting the constants to unity. Either equation now gives

$$\frac{1}{\tau_I} = \frac{\frac{\alpha_I}{\tau_{I0}} + \frac{\alpha_C}{\tau_{C0}}}{1 + \alpha_I + \alpha_C} . \quad (6.11)$$

This equation gives the damping time for diffusion between regions in terms of the damping times for diffusion out of the regions and the fractions α .

In the solutions (6.8) the second terms are negligible compared with the gaussian first terms except near the boundaries. The solution is therefore

normalized to one particle in the islands and minus one in the central triangle. The total number of particles is zero, as it must be if the solution is to be damped and still conserve total particle number.

We can now find the solution corresponding to N particles initially in the central triangle and none in the islands. The final state is given by Eqs.(6.2) and (6.6). To get the initial state, multiply the normalized damped solution (6.6) above by $-N_I$ and add it to the solution (6.2). This gives the initial state except for small terms near the boundaries. As the damped solution dies away with time constant τ_1 the solution approaches the equilibrium solution (6.2). Except near the boundaries, the solution in each region is essentially a gaussian which dies out exponentially in the central triangle and grows exponentially in the islands. A similar solution can be found for the case where the beam is initially in the islands.