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Chaotic Mixing in Charged-Particle Beams

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Abstract

For a charged-particle bunch with external focusing and internal space charge that together produce globally chaotic orbits, the e-folding time by which an initially localized ensemble of chaotic orbits irreversibly disperses globally through the bunch is estimated. The density distribution determines how rapidly this mixing, with associated macroscopic changes in the bunch structure, proceeds. The theory also applies to self-gravitating systems; it is tested against recent simulations of chaotic mixing in elliptical galaxies having a massive black hole at their centroids.

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Rapid irreversible dynamics is a practical concern in producing high-brightness charged-particle beams. Time scales of irreversible processes place constraints on methods for compensating against degradation of beam quality caused by, for example, space charge in high-brightness injectors [1] or coherent synchrotron radiation in accelerators that power modern free-electron lasers [2]. Compensation needs to be fast compared to active irreversible processes, which in turn affects the choice and configuration of the associated hardware.

A beam bunch with space charge comprises an N-body system with typically $3N$ degrees of freedom. The particle trajectories are generically chaotic due, at minimum, to granularity in the space-charge potential. Through a process known as "chaotic mixing" [3], an initially localized ensemble of chaotic orbits will grow exponentially and eventually diffuse through its accessible phase space, reaching an invariant distribution. The process is irreversible in the sense that infinitesimal fine-tuning is needed to reassemble the initial conditions. It is also distinctly different from phase mixing, a process that winds an initially localized ensemble into a filament over a comparatively narrow region of phase space, and that is in principle reversible. Whereas chaotic mixing proceeds exponentially over a well-defined time scale and causes global, macroscopic changes in the system, phase mixing carries an algebraic time dependence, proceeds on a time scale depending on the distribution of orbital frequencies across the ensemble, and acts only over a portion of the phase space.

Chaotic mixing may or may not be rapid. For example, simulations of large self-gravitating N-body systems in which the smoothed density is constant over a stationary ellipsoidal volume show that the orbits, though they are chaotic, behave for very long times as if they were regular [4]. These simulations, however, also reveal that adding a density cusp and/or inserting a massive black hole at the centroid can greatly accelerate chaotic mixing, driving it to completion within a few orbital periods. The process tends to make the distribution of stars more isotropic [5], reminiscent of equipartitioning in beams. In short, structure in the density distribution of a self-gravitating system can lead to rapid chaotic mixing by increasing the degree of chaoticity of the orbits.

By analogy, one might conjecture that structure in the density distribution of a selfinteracting beam can likewise lead to rapid chaotic mixing. One example is the University of Maryland five-beamlet experiment that showed irreversible dissipation of the beamlets after a few space-charge-depressed betatron periods [6]. Simulations of the experiments revealed a substantial fraction of globally chaotic orbits [7], and chaotic mixing thereby presents itself as a possible mechanism. Moreover, rapid irreversible mixing is also seen in recent simulations of merging multiple beamlets in accelerators for heavy-ion fusion [8]. In any case, ascertaining conditions that lead to rapid chaotic mixing in beams is an undertaking of practical importance.

The past few years have seen development of a geometric method proposed by M. Pettini to quantify chaotic instability in Hamiltonian systems with many degrees of freedom. The central idea is to describe the dynamics in terms of average curvature properties of the manifold in which the particle orbits are geodesics. The method hinges on the following assumptions and approximations, which are discussed thoroughly in Ref. [9]: (1) a generic geodesic is chaotic; (2) the manifold's effective curvature is locally deformed but otherwise constant; (3) the effective curvature reflects a gaussian stochastic process; and (4) long-time-averaged properties of the curvature are calculable as phase-space averages over an invariant measure, specifically, the microcanonical ensemble. The gaussian process is the zeroth-order term in a cumulant expansion of the actual stochastic process; assumption (3) is that the zeroth-order term suffices. The end result relates chaotic instability to the geometric properties of the manifold defined by the long-time-averaged orbits. Though the assumptions and approximations lack universal validity and are difficult to prove rigorously for a given system, they nonetheless would seem to offer a reasonable basis for identifying conditions that can produce rapid chaotic mixing. Our goal here is to apply the method of Ref. [9] to infer an analytic expression for the mixing time, first in a stationary beam bunch with space charge, and second in a family of self-gravitating systems for comparison to the aforementioned simulations.

Action principles in classical mechanics are tantamount to extremals of "arc lengths"; thus, one can infer a metric tensor from an action principle [10]. The metric tensor manifests all of the properties of the manifold over which the system evolves, with these properties being calculable following standard principles of differential geometry. Of special interest is the divergence of two initially nearby $3N$-dimensional geodesics $\mathbf{q}$ and $\mathbf{q}+\delta\mathbf{q}$ as governed by the equation of geodesic deviation:

$$\frac{D^2\delta q^\alpha}{ds^2} + R^\alpha{}_{\beta\gamma\delta}\frac{dq^\beta}{ds}\delta q^\gamma\frac{dq^\delta}{ds} \;=\; 0, \tag{1}$$

in which D/ds denotes covariant differentiation with respect to the "proper time" s, $R^\alpha{}_{\beta\gamma\delta}$ is the Riemann tensor derivable from the metric tensor, and summation over repeated indices is implied with each index spanning the $3N$ degrees of freedom. Equation (1) is the basis for determining the mixing rate λ as a measure of the system's largest Lyapunov exponent, a quantity that reflects the long-time behavior of the separation vector:

$$\lambda \;=\; \lim_{t\to\infty}\frac{1}{t}\ln\frac{|\delta\mathbf{q}(t)|}{|\delta\mathbf{q}(0)|}. \tag{2}$$

Any number of action principles, and therefore any number of metric tensors, can be selected to proceed further. Eisenhart's metric [11], which is consistent with Hamilton's least-action principle, is probably the most convenient choice. It offers easy calculation of the Riemann tensor, and it avoids spurious results traceable to the singular boundary of the perhaps better-known Jacobi metric that is derivable from Maupertius' least-action principle [12]. Eisenhart's metric operates over an enlarged configuration space-time manifold in which the geodesics are parameterized by the real time t, *i.e.*, $ds^2 = dt^2 = -2V(\mathbf{q})(dq^0)^2 + \delta_{ij}dq^i dq^j + 2dq^0 dq^{3N+1}$, in which $V(\mathbf{q})$ is the potential energy per unit mass (hereafter called the "potential"), δ_{ij} (with the indices i, j running from 1 to $3N$) is the unit tensor corresponding (without loss of generality) to a cartesian spatial coordinate system, $q^0 = t$, $q^{3N+1} = t/2 - \int_0^t dt' L(\mathbf{q}, \dot{\mathbf{q}})$, and L is the Lagrangian. The resulting geodesic equations for the spatial coordinates q^i are Newton's equations of motion, so the particle trajectories correspond to a canonical projection of the Eisenhart geodesics onto the configuration space-time manifold. A convenient byproduct of the Eisenhart metric is that the only nonzero components of the Riemann tensor are $R_{0i0j} = \partial_i\partial_j V$, in which $\partial_i = \partial/\partial q^i$.

Using the aforementioned assumptions and approximations, Pettini and others [9,13] derive an expression for λ in terms of the curvature and its standard deviation averaged over the microcanonical ensemble. The idea is that, as $t \to \infty$, chaotic orbits of total energy E mix through the configuration space toward an invariant measure, taken per assumption (4) to be the microcanonical ensemble $\delta(H-E)$, over which time averages become equivalent to phase-space averages. Specifically, for an arbitrary function $A(\mathbf{q})$, the averaging process is

$$\langle A\rangle \equiv \lim_{t\to\infty}\langle A\rangle_t = \frac{\int d\mathbf{q}\int d\dot{\mathbf{q}}\; A(\mathbf{q})\delta[H(\mathbf{q},\dot{\mathbf{q}})-E]}{\int d\mathbf{q}\int d\dot{\mathbf{q}}\; \delta[H(\mathbf{q},\dot{\mathbf{q}})-E]}. \tag{3}$$

Per Eisenhart's metric, the average curvature and standard deviation are, respectively,

$$\kappa = \frac{\langle\Delta V\rangle}{3N-1}, \quad \sigma = \sqrt{\frac{\langle(\Delta V)^2 - \langle\Delta V\rangle^2\rangle}{3N-1}}, \tag{4}$$

in which Δ denotes the Laplacian $\partial_i\partial^i$. Pettini *et. al.*'s method yields

$$\begin{aligned}\lambda(\rho) &= \frac{1}{\sqrt{3}}\frac{L^2(\rho)-1}{L(\rho)}\sqrt{\kappa};\\ L(\rho) &= \left[T(\rho)+\sqrt{1+T^2(\rho)}\right]^{1/3}, \quad T(\rho) = \frac{3\pi\sqrt{3}}{8}\frac{\rho^2}{2\sqrt{1+\rho}+\pi\rho};\end{aligned} \tag{5}$$

in which $\rho \equiv \sigma/\kappa$, a quantity that measures the ratio of the average curvature radius to the length scale of fluctuations [14]. For small ρ, $\lambda/\kappa^{1/2}$ scales as ρ^2, and for large ρ it scales as $\rho^{1/3}$.

The geometric quantities derive from the $6N$-dimensional microcanonical ensemble. Anticipating that granularity takes a long time to affect mixing, and wishing to identify conditions for rapid mixing, we now consider the influence of the 3-dimensional coarse-grained space-charge potential V_s on a generic chaotic orbit. We presume the assumptions and approximations stated at the outset carry over to the coarse-grained system; when they do not, chaotic mixing will normally be too slow to be of concern. We take the external focusing potential V_f to be quadratic in the coordinates $\mathbf{x}$ comoving with the bunch, *i.e.*, $V_f(\mathbf{x}) = (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2$; the total potential is $V = V_f + V_s$. Per Eq. (4) and Poisson's equation the quantities κ and σ are determined from $\nabla^2 V = \omega_f^2 - \omega_p^2(\mathbf{x})$, in which $\omega_f^2 = \omega_x^2 + \omega_y^2 + \omega_z^2$, $\omega_p^2(\mathbf{x}) = n(\mathbf{x})e^2/(\epsilon_o m)$, $n(\mathbf{x})$ is the (smoothed) particle density, e and m are the single-particle charge and mass, respectively, and ϵ_o is the permittivity of free space. With $\omega_{p0} \equiv \omega_p(0)$, the results may be expressed conveniently in terms of the space-charge-depressed focusing strength $\omega_s^2 = \omega_f^2 - \omega_{p0}^2$ and the normalized particle density $\nu(\mathbf{x}) = n(\mathbf{x})/n(0)$ as $\kappa = (\omega_{p0}^2/2)\left[(\omega_s/\omega_{p0})^2 + 1 - \langle\nu\rangle\right]$, $\sigma = \omega_{p0}^2\sqrt{(\langle\nu^2\rangle - \langle\nu\rangle^2)/2}$. Inserting these results into Eq. (5) gives the associated time scale, $t_m \equiv 1/\lambda$, for irreversible chaotic mixing. When the standard deviation of the density distribution is large, as can be the case when substructure is present, ρ will be appreciable, and in turn Eq. (5) makes clear that t_m will be a few space-charge-depressed betatron periods. This is consistent with, *e.g.*, the aforementioned University of Maryland experiment showing irreversible dissolution of both matched and mismatched 5-beamlet configurations over a few depressed betatron periods [6].

The aforementioned studies in galactic dynamics permit a quantitative test of the theory. Simulations of chaotic mixing in galaxies consisting of a homogeneous ellipsoid with a density cusp and/or a massive black hole at its centroid have recently been done, such as those of Siopis and Kandrup [15] (hereafter SK) and Valluri and Merritt [4] (hereafter VM). SK show that these simulations can be considered in the context of a simple "toy" potential, namely

$$V(\mathbf{q}) \;=\; \frac{1}{2}\left(\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}\right) \;-\; \frac{M}{\sqrt{r^2+\epsilon^2}}, \tag{6}$$

wherein M denotes the black-hole mass, ϵ is a parameter that softens close encounters with the black hole, and the semiaxes are $a = 2/\sqrt{3}$, $b = 1$, $c = 2/\sqrt{5}$. The density and mass of the homogeneous ellipsoid are, respectively, $3/(4\pi)$ and $4/\sqrt{15} \simeq 1$. The simulations start with an ensemble of test particles, each having zero initial velocity, distributed over a localized portion of an equipotential of energy E. The particles respond to the potential and do not interact with each other. SK discuss the ensemble's distribution of Lyapunov exponents, and VM discuss the e-folding time of the expansion of the ensemble due to chaotic mixing. Whereas SK explicitly use the toy potential for their simulations that are discussed below, VM's potential has an additional shallow density cusp at the centroid. Following SK's suggestion, we still use the toy potential to interpret VM's results.

Phase-space averages are straightforwardly evaluated per Eq. (3), *e.g.*, by first doing the easy integral over velocity space, then rewriting the new integrands in terms of confocal ellipsoidal coordinates, and finally integrating over the volume of the ellipsoid. It turns out that κ and σ are mathematically insensitive to the ellipsoidal geometry, *i.e.*, to the ellipticity, and spherically symmetric models of the integrands give essentially the same results. This simplification facilitates developing the following closed-form approximation for the mixing time t_m that reveals the parametric scaling with black-hole mass M and particle energy E:

$$t_m = \frac{3\sqrt{3}}{2T(\rho)\sqrt{\kappa}}; \quad \rho = \frac{3\sqrt{5}}{2^{13/4}}\frac{M}{\kappa\epsilon^{3/2}E^{3/4}}, \quad \kappa = \frac{3\pi E^{3/2}+4\sqrt{2}M}{2\pi E^{3/2}}, \tag{7}$$

and $T(\rho)$ is as given in Eq. (5). SK explicitly list the particle energies E in their ensembles. VM start their ensembles on equipotentials enclosing a mass of the ellipsoid without the black hole that is approximately a multiple $n = 3, 7, 17$ of the black-hole mass; corresponding energies for use with the toy potential may be estimated from a spherically symmetric model of the potential as $E_n \simeq [(n/2) - 1](M^2/n)^{1/3}$.

Theoretical mixing times τ_{th}, calculated from Eq. (7) with the softening parameter set at $\epsilon = 0.16$ (for reasons discussed below), are given in Table 1. Per VM's convention, the mixing times are normalized to each ensemble's crossing time t_c, *i.e.*, $\tau \equiv t_m/t_c$, with t_c defined as half the orbital period along the semimajor axis as calculated from the potential in the absence of the black hole. For the toy potential, the crossing time is, accordingly, $t_c = \pi a = 2\pi/\sqrt{3}$. Normalized mixing times τ_{sim} deriving from the simulations are also given in Table 1. Those quoted for SK derive from their Fig. 19 and correspond to the peaks in the distributions of Lyapunov exponents for the respective ensembles. Those quoted for VM derive from their Fig. 4. For their lowest-energy ensemble, VM state that the linear extent of the points in configuration space doubles roughly each crossing time until the ensemble has essentially filled its accessible volume. The associated e-folding time is thus $\tau \simeq 1/\ln 2 = 1.4$, and VM's Fig. 4 shows the mixing times for the other two ensembles are factors of $\sim 13/8$ and $\sim 24/8$ larger.

The normalized mixing times calculated from theory track those inferred from the simulations over the considerable range of parameters reflected in Table 1. Moreover, VM find that mixing becomes markedly slower as the black-hole mass is reduced below $M \sim 0.01$, another quantitative result that Eq. (7) reproduces. These findings point to the theory's utility and also imply that the normalized mixing time is insensitive to minor refinements in the potential, such as VM's shallow density cusp. However, there is an important limitation: the theory depends on a "free parameter", namely the softening parameter ϵ, the presence of which reflects uncertainty about the detailed dynamical properties of the phase space. As concerns the toy potential, one knows *a priori* that far from M it is approximately quadratic in the coordinates, and close to M it is approximately spherically symmetric; the orbits are accordingly quasiregular in these regions wherein there will be almost no chaotic mixing. The theory correctly predicts zero mixing in a harmonic-oscillator potential, thereby incorporating the former circumstance, but it also incorrectly predicts nonzero mixing in a spherically symmetric potential like that close to M. Thus, a nonzero ϵ "regularizes" orbits near the black hole. The parametric scaling of τ_{th} is insensitive to ϵ, but its magnitude is sensitive, and the choice $\epsilon = 0.16$ gives magnitudes consistent with those of the simulations.

As concerns charged-particle beams, establishing general criteria by which space charge induces globally chaotic orbits is a goal of contemporary work. When chaotic mixing is active, structure in the density distribution determines how rapidly it progresses. Production of high-brightness beams may lead to transient, localized density peaks, as has been seen, *e.g.*, during bunch compression [16] and in merging multiple beamlets [6,8]. Thus, an accelerator designer who cannot know *a priori* the detailed bunch structure will want to ensure that emittance compensation is completed within roughly a plasma period to be confident that irreversible mixing will not spoil the compensation. This criterion translates into permissible beamline locations and maximum lengths that the associated hardware can occupy [17].

Because it is based on the Eisenhart metric, the present treatment is restricted to stationary systems. However, with a Finsler metric, the geometric method can also incorporate potentials that are explicitly time-dependent and/or velocity-dependent [18]. For example, recent work involving the Hénon-Heiles potential [19] resulted in a geometric measure of chaos over the associated Finsler manifold that was used for fast computation of the system's Poincaré surface of section. By analogy, one is led to suspect that this technique may likewise yield efficient calculation of dynamic apertures in circular machines in which magnet nonlinearities, and perhaps beam-beam interactions, gradually degrade the beam. The principal advantage would be circumvention of very long integration times and their attendant numerical difficulties. If used with a coarse-grained potential, the Eisenhart metric includes no mechanism for changing the particle energies and thereby excludes important processes such as violent relaxation and attendant halo formation [20]. In principle, they can be included with a Finsler metric based on a time-dependent coarse-grained potential; however, the generalization also requires specifying a suitable invariant measure for the nonequilibrium system [21].

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TABLES

Table 1. Galactic Mixing Times: Theory vs. Simulation

Authors	M	E	τ_{th}	τ_{sim}
SK	$10^{-3/2}$	0.044	1.4	1.4
SK	0.01	0.065	5.2	5.5
VM	0.03	0.033	1.4	1.4
VM	0.03	0.13	2.2	2.3
VM	0.03	0.28	4.2	4.3