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NONPERTURBATIVE GEOMETRODYNAMIC CALCULATION OF CHAOTIC MIXING TIME IN CHARGED-PARTICLE BEAMS

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The time scale for irreversible mixing in a charged-particle bunch as a consequence of time-independent, nonlinear space-charge forces is estimated analytically to be a few plasma periods, much shorter than the two-body relaxation time. The basis for the estimate is a metric tensor inferred from Hamilton's least-action principle. Geodesics derived from the metric tensor correspond to particle trajectories. Their behavior reflects the properties of the curvilinear manifold in which they are embedded, among which irregularities associated with parametric resonances are of foremost importance. Exponential separation of nearby chaotic trajectories is thereby accessible to the geometrodynamic approach. The e-folding time associated with dispersing an initially localized perturbation throughout the bunch characterizes the process of irreversible mixing. It thereby constrains both the placement and size of hardware for emittance compensation that may be needed, for example, to undo phase-space degradation arising from coherent synchrotron radiation in magnetic bends. These constraints are estimated for linacs powering modern infrared and x-ray free-electron lasers.

1 Introduction

The past six years have seen the development of a geometrodynamic technique for analytically estimating the largest Lyapunov exponent in a system having many degrees of freedom. A comprehensive synopsis of the work appears in a new preprint posted subsequent to this Workshop.[1] The technique permits consideration of chaotic orbits that mix through the configuration space on an exponential time scale. The mixing is irreversible in the sense that infinitesimally small fine-tuning is needed to reassemble the initial conditions. It is also distinctly different from phase mixing (linear Landau damping), a regular, reversible process that "winds up" the phase space through a distribution of orbital frequencies. Phase mixing proceeds on a relatively slow time scale set by the distribution of frequencies.

Based on geometrodynamics, this paper presents an estimate of the time scale for chaotic mixing in a charged-particle bunch under the influence of nonlinear space-charge forces. The time scale is used to infer constraints on emittance-compensation schemes, particularly those related to undoing the effects of coherent synchrotron radiation in accelerators that power modern free-electron lasers. Although key aspects of the geometrodynamic technique are discussed herein, the interested reader is referred to Ref. 1 for details and further discussion.

2 Preliminaries

Space charge will typically result in a nonintegrable potential, *i.e.*, one in which the degrees of freedom are coupled. Systems having at least two degrees of freedom and a nonintegrable potential can be expected to comprise a significant percentage of chaotic orbits. This is true even if the potential is in a stationary state.

We consider a charged-particle bunch governed by an autonomous (time-independent) Hamiltonian in which space charge is active. We formulate the problem with respect to a reference frame comoving with the bunch; the origin of the reference frame coincides with the centroid of the bunch. Calculated time scales are then Lorentz-transformed to the laboratory frame.

On a global scale, the bunch will generally be three-dimensional and have a density distribution exhibiting a Debye tail.[2] Interior particles that never reach into the Debye tail are effectively screened from external forces; however, particles reaching into the Debye tail will respond to these forces and communicate their influence throughout the bunch. Nonlinear space-charge forces likewise predominate in the Debye tail, so these same particles are also the ones that are most susceptible to chaotic behavior. Moreover, on a local scale, a bunch is fully $3N$-dimensional, with N representing the number of particles. All of the constituent particles are therefore under the influence of local space-charge fluctuations, and conditions can be such that a generic orbit is chaotic. That nonlinear space-charge forces establish chaotic orbits is evident in, for example, many of the papers in these Proceedings.

We now turn attention toward calculating the time scale for mixing. Action principles in classical mechanics are tantamount to extremals of "arc lengths;" thus, one can infer a metric tensor from an action principle.[3] 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.[4] Of special interest for determining Lyapunov exponents, quantities that measure the exponential rate at which initially localized trajectories separate, is 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 $\mathbf{q}(s)$ denotes the coordinate vector of the system, $\delta\mathbf{q}(s)$ represents the separation vector between neighboring geodesics at "proper time" s, D/ds denotes covariant differentiation, $R^{\alpha}{}_{\beta\gamma\delta}$ is the Riemann tensor derivable from the metric tensor, and summation over repeated indices is implied with each index spanning the number of degrees of freedom accessible to the system. Equation (1) is fundamental for determining a Lyapunov exponent λ because it is defined in terms 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, which is consistent with Hamilton's least-action principle, is probably the most convenient choice.[5] It offers what is probably the easiest 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.[6] Eisenhart's metric operates over a combined space-time manifold in which the geodesics are parameterized by the real time t, *i.e.*, $ds^2 = dt^2$ with

$$ds^2 \;=\; -\,2V(\mathbf{q})(dq^0)^2 + \delta_{ij}dq^i dq^j + 2dq^0 dq^{\mathcal{N}+1}, \tag{3}$$

in which $V(\mathbf{q})$ is the potential, δ_{ij} is the unit tensor corresponding (without loss of generality) to a cartesian spatial coordinate system, the indices i, j run from 1 to the number of degrees of freedom $\mathcal{N}$ ($= 3N$ generally), $q^0 = t$, $q^{\mathcal{N}+1} = t/2 - \int_0^t dt' L(\mathbf{q},\dot{\mathbf{q}})$, and L is the Lagrangian. The resulting geodesic equations for the spatial coordinates q^i are Hamilton's equations of motion, so the particle trajectories correspond to a canonical projection of the Eisenhart geodesics onto the configuration's 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 $\partial_i = \partial/\partial q^i$. In turn, the only nonzero component of the Ricci tensor $R_{\alpha\beta} \equiv R^{\gamma}{}_{\alpha\gamma\beta}$ is $R_{00} = \partial^i\partial_i V$.

3 Generic Geodesic Deviation

Rather than evaluate the geodesic deviation along all possible directions, we instead construct and study a generic geodesic deviation. To set up the governing equation, we put $\delta\mathbf{q} \propto \sqrt{\psi}\hat{\mathbf{n}}$, with $\hat{\mathbf{n}} = \delta\mathbf{q}/|\delta q|$ denoting the unit vector. Then, recognizing that there is no exponential growth of a deviation that is parallel to the geodesic, we average the equation of geodesic deviation (1) over all $\mathcal{N}-1$ perturbations $\delta\mathbf{q}$ that are orthogonal to the reference geodesic. The resulting equation of "generic" geodesic deviation is[7]

$$\frac{d^2\psi}{dt^2} + \frac{\mathcal{H}^\beta{}_\beta}{\mathcal{N}-1}\psi \;=\; 0, \tag{4}$$

in which $\mathcal{H}^\beta{}_\beta = R_{\mu\nu}\dot{q}^\mu\dot{q}^\nu = \partial^i\partial_i V$ measures the curvature of the manifold along the geodesics, *i.e.*, the particle trajectories. Although the potential $V(\mathbf{q})$ is taken to be explicitly time-independent, the "curvature" $\mathcal{H}^\beta{}_\beta = \partial^i\partial_i V$ nevertheless depends on time because it is measured with reference to the geodesics that are parameterized by the time t. The potential is a function of the coordinate vector $\mathbf{q}(t)$, which in turn is implicitly time-dependent.

4 Stochastic Influence of Parametric Resonances

As they flow over the manifold, each particle will respond to the "bumpiness," *i.e.*, the local curvature, it sees, the bumpiness being associated with parametric resonances between the instantaneous orbital period and the effective nonlinear forces. For a chaotic orbit we regard the resonances to act stochastically, and we take the equation of generic geodesic deviation to be that of a stochastic oscillator:

$$\frac{d^2\psi}{dt^2} + \left[\kappa_t + \sigma_t\eta(t)\right]\psi \;=\; 0, \tag{5}$$

in which κ_t and σ_t are related to the time-averaged curvature and fluctuations, respectively:

$$\kappa_t \;=\; \frac{\langle\mathcal{H}^\beta{}_\beta\rangle_t}{\mathcal{N}-1}; \quad \sigma_t = \frac{\sqrt{\left\langle(\mathcal{H}^\beta{}_\beta)^2 - \langle\mathcal{H}^\beta{}_\beta\rangle_t^2\right\rangle_t}}{\sqrt{\mathcal{N}-1}}, \tag{6}$$

and $\eta(t)$ denotes a gaussian stochastic process. Specifically, $\langle\eta(t)\eta(t-\tau)\rangle = \tau\delta(t)$, where the average is taken over all realizations of the process, and τ is the correlation time, which is intermediate between the time required for the particle to traverse the average curvature radius and the time for it to transit the length scale of a typical fluctuation.[9] A gaussian process is the zeroth-order approximation of a cumulant expansion of the actual stochastic process.

As $t \to \infty$, which is the limit of interest for calculating a Lyapunov exponent, orbits of total energy E that mix through the configuration space will evolve toward an invariant measure, specifically the microcanonical ensemble $\mu = \delta(H - E)$, over which time averages become equivalent to phase-space averages. Given our expectation that space charge will typically establish a preponderance of chaotic orbits, we therefore consider it a reasonable approximation to average over the microcanonical ensemble, which is tantamount to invoking the so-called "chaotic hypothesis".[8] Accordingly, for an arbitrary function $A(\mathbf{q})$ of the spatial coordinate $\mathbf{q}$, the average becomes

$$\lim_{t\to\infty}\langle A\rangle_t \;=\; \langle A\rangle_\mu \;=\; \frac{\int d\mathbf{q}\int d\dot{\mathbf{q}}\; A(\mathbf{q})\delta[H(\mathbf{q},\dot{\mathbf{q}})-E]}{\int d\mathbf{q}\int d\dot{\mathbf{q}}\; \delta[H(\mathbf{q},\dot{\mathbf{q}})-E]}, \tag{7}$$

and the generic geodesic approximately adheres to the simplified stochastic-oscillator equation

$$\frac{d^2\psi}{dt^2} + [\kappa + \sigma\eta(t)]\,\psi \;=\; 0, \tag{8}$$

in which κ, σ is shorthand notation for $\langle\kappa\rangle_\mu$, $\langle\sigma\rangle_\mu$. Note that all averages $\langle A\rangle_\mu$ are evaluated for a given total particle energy E; the averages are therefore functions of particle energy.

Van Kampen[10] devised a method for calculating from Eq. (8) the evolution of the process-averaged second moments of ψ, out of which the Lyapunov exponent corresponding to the mixing rate appears as a function of the correlation time τ.[9] Using a reasonable estimate of τ, one can write the Lyapunov exponent in the following convenient analytical form:

$$\begin{aligned}
\lambda(\rho) \;&=\; \frac{1}{\sqrt{3}}\frac{L^2(\rho)-1}{L(\rho)}\sqrt{\kappa};\\
L(\rho) \;&=\; \left[T(\rho)+\sqrt{1+T^2(\rho)}\right]^{1/3}, \;\; T(\rho) \;=\; \frac{3\pi\sqrt{3}}{8}\frac{\rho^2}{2\sqrt{1+\rho}+\pi\rho};
\end{aligned} \tag{9}$$

in which $\rho \equiv \sigma/\kappa$, a quantity that measures the ratio of the average curvature radius to the length scale of fluctuations.[11] A plot of $\lambda/\sqrt{\kappa}$ versus ρ is given in Fig. 1; the plot makes clear that the time scale for mixing, $1/\lambda$, is a ρ-dependent multiple of $\kappa^{-1/2}$, so that $\kappa^{-1/2}$ is the fundamental time scale governing the irreversible process. Near the origin the curve scales as ρ^2, and at large ρ it scales as $\rho^{1/3}$.

There are seemingly several approximations leading to Eq. (9); however, they are all summarized concisely by the notion that a generic trajectory is chaotic, governed by a gaussian random process under the influence of parametric resonances, and evolves toward an invariant measure that is the microcanonical ensemble. Numerical experiments, principally concerning condensed matter and stellar systems, historically guided the thinking that led to the estimate. For example, Ref. 1 summarizes simulations of coupled-spin systems with long-range interactions and shows the analytically estimated Lyapunov exponents agree remarkably well with computed values. We are

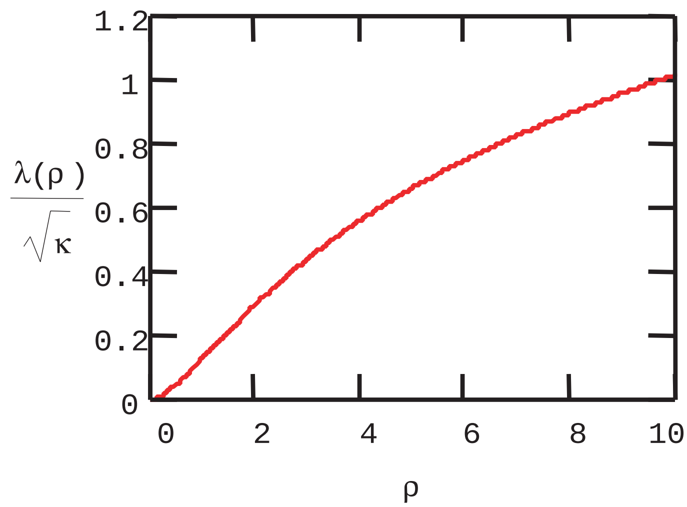

Figure 1. Lyapunov exponent in units of $\sqrt{\kappa}$ plotted as a function of $\rho = \sigma/\kappa$; the quantities κ and σ are defined in the text.

therefore led to inquire what the method will predict concerning the influence of space charge in beams.

5 Application to Beams with Space Charge

5.1 Time Scale for Onset of Irreversibility

We presume that when space charge is important, it influences a given particle trajectory primarily through a coarse-grained potential that is everywhere proportional to the local particle density. Consequently, we shall apply the foregoing results to a single charge that orbits in a smooth, three-dimensional ($\mathcal{N} = 3$) potential $V = V_o + V_s$, with V_o denoting the potential associated with focusing forces external to the bunch, and V_s denoting the coarse-grained potential associated with space-charge forces internal to the bunch. For concreteness we take the external forces to be linear so V_o is quadratic in the coordinates, *i.e.*, $V_o(\mathbf{q}) = (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2$. Application of Poisson's equation then gives a simple result:

$$\nabla^2 V \ = \ \omega_o^2 - \frac{e}{\epsilon_o} n(\mathbf{q}), \tag{10}$$

in which $\omega_o^2 = \omega_x^2 + \omega_y^2 + \omega_z^2$, e is the single-particle charge, ϵ_o is the permittivity of free space, and $n(\mathbf{q})$ is the particle density.

The quantities κ and σ are both determined from the Laplacian of the coarse-grained potential. It is convenient to express the results in terms of the plasma frequency at the bunch centroid, ω_{po}, the "reduced" focusing strength $\omega_s^2 = \omega_o^2 - \omega_{po}^2$, and the normalized particle density $\nu(\mathbf{q}) = n(\mathbf{q})/n(0)$:

$$\begin{aligned}
\kappa &= \frac{\omega_{po}^2}{2}\left[\left(\frac{\omega_s}{\omega_{po}}\right)^2 + 1 - \langle\nu\rangle\right], \\
\sigma &= \frac{\omega_{po}^2}{\sqrt{2}}\sqrt{\langle\nu^2\rangle - \langle\nu\rangle^2}, \\
\rho &= \frac{\sigma}{\kappa} = \frac{\sqrt{2}\sqrt{\langle\nu^2\rangle - \langle\nu\rangle^2}}{(\omega_s/\omega_{po})^2 + 1 - \langle\nu\rangle}. \qquad (11)
\end{aligned}$$

From the estimated Lyapunov exponent as given by Eq. (9), one sees that the time scale for chaotic mixing and its associated irreversibility, $\tau_m \equiv 1/\lambda$, is principally determined by the value of $1/\sqrt{\kappa}$ and is modified in the prescribed way by the value of ρ which carries the influence of the operative parametric resonances. Equation (11) makes clear that τ_m is a multiple of the plasma period $\tau_p \equiv 2\pi/\omega_{po}$. In realistic inhomogeneous density distributions, the value of ρ will typically be small but appreciable, and in turn Fig. 1 makes clear that τ_m will typically be a few plasma periods. Thus, as concerns guarding against the deleterious influence of space charge on a process of emittance compensation, a reasonable conservative criterion is to ensure the process is completed within a plasma period.

5.2 Reversibility Criterion vs. Beam Parameters

The criterion that emittance compensation be done within a plasma period carries implications for the location and size of the associated hardware. For example, there are several options for reversing or minimizing emittance growth from coherent synchrotron radiation (CSR) in magnetic bends.[12] One of them is to add magnetic optics as a source of dispersion to undo the CSR-induced bunch distortion. Our criterion implies the associated hardware would need to be contained inside a length $L < \beta c \tau_p$. The objective here is to express this constraint in terms of beam parameters.

The plasma frequency can be expressed in the laboratory frame in terms of the total bunch charge Q, the particle rest mass m, and the root-mean-square widths $\tilde{x}, \tilde{y}, \tilde{z}$ of the density profile as follows:[13]

$$\omega_p \;=\; \frac{1}{\gamma^{3/2}}\sqrt{\frac{3Qe}{20\pi\sqrt{5}\epsilon_o m\tilde{x}\tilde{y}\tilde{z}}}, \tag{12}$$

from which the plasma period is simply $\tau_p = 2\pi/\omega_p$. The constraint $L < \beta c\tau_p$ thereby imposes a corresponding constraint on the particle kinetic energy $T = (\gamma - 1)mc^2$ above which the emittance compensation should succeed:

$$\frac{T}{mc^2} \;>\; \left(\frac{L}{\beta}\right)^{2/3}\left(\frac{3Qe}{80\pi^3\sqrt{5}\epsilon_o mc^2\tilde{x}\tilde{y}\tilde{z}}\right)^{1/3} - 1. \tag{13}$$

Specialized to a bunched electron beam ($\beta \sim 1$), and written in units representative of modern high-brightness electron linacs, this constraint becomes

$$T(\mathrm{MeV}) \;>\; 2.5\left\{\frac{Q(\mathrm{nC})[L(\mathrm{m})]^2}{\tilde{x}(\mathrm{mm})\tilde{y}(\mathrm{mm})\tilde{z}(\mathrm{mm})}\right\}^{1/3} - 0.511. \tag{14}$$

5.3 Example: Linacs for Free-Electron Lasers

High-brightness linacs are generally required for free-electron lasers (FELs) that are intended to produce high-average-power coherent light and/or short wavelengths. The essential requirement is to confine the electrons comprising the high-charge bunch to within the optical mode through the undulator so that they all, or nearly all, participate in the lasing process. Examples are Jefferson Laboratory's infrared FEL (the "IR Demo") for which commissioning was completed in summer 1999 resulting in sustained 1.7 kW average continuous-wave power at wavelengths in the range 3-6 μm,[14] and x-ray FELs presently under development at SLAC and DESY.[15] In both cases CSR-induced emittance degradation is a concern, although the IR Demo was designed to circumvent the influence of CSR on lasing while still providing a platform for CSR-related experiments. To get some numbers, we shall imagine that hardware for emittance compensation spans $L = 5$ m, a nominal length scale for a chicane of dipole magnets.

Typical beam parameters for the IR Demo are $Q \sim 0.1$ nC, $T \leq 48$ MeV, and $\tilde{x} \sim \tilde{y} \sim \tilde{z} \sim 1$ mm; whereas typical beam parameters in linacs for x-ray FELs will be $Q \sim 1$ nC, $T \leq 1$ GeV, and $\tilde{x} \sim \tilde{y} \sim \tilde{z} \sim 0.1$ mm. Thus, to avoid space-charge-driven chaotic mixing and its associated irreversibility, the hardware would need to be placed at $T > 3$ MeV in the IR Demo, or $T > 70$ MeV in the x-ray FELs. By comparison, the IR Demo injector delivers 10 MeV beam, which is to say compensation could be done anywhere after the injector. In the case of x-ray FELs, bunch compression/compensation appears viable as long as it is done not too close to the front end of the machine.

6 Summary and Discussion

Using geometrodynamics we found that the fundamental time scale for chaotic mixing induced by nonlinear space-charge forces in a stationary beam bunch is the plasma period ω_p. Because the process is macroscopically irreversible, emittance compensation needs to be done within this time scale to be most effective.

The mixing time is very short compared to the collisional relaxation time. The latter scales roughly as N_D/ω_p, where N_D is the number of particles in a Debye sphere. The collisional relaxation time in a beam with space charge is thus typically a factor $\sim N_D$, *i.e.*, several orders of magnitude, larger than the mixing time.

The mixing time calculated here differs from a relaxation time. For example, the geometrodynamic treatment based on Eisenhart's metric takes no account of the evolution of velocity space. Moreover, the use of a coarse-grained potential in the calculation washes out the influence of collisions. Although we have specialized to beams with space charge, we may nevertheless infer that, for a system in which parametric resonances cause typical particle trajectories to be chaotic, the mixing time will be governed principally by a global time scale derivable from the Lagrangian of the potential. Thus the time scale of interest in plasmas is the plasma period, in gravitational systems it is the free-fall time, etc.

In discussing a mixing time, one must take care to do so in terms of globally chaotic behavior of the system. In other words, an initially localized perturbation may be regarded to have mixed only after it has grown to the point that its scale is comparable to the size of the system. By contrast, noise associated with single-particle interactions can also generate rapid exponential growth of perturbations, but the growth saturates on small scales and is therefore not representative of mixing.[16]

Our calculation has the attractive feature of being focussed on the behavior of a generic, *i.e.*, "average" trajectory that samples the global phase space established by a coarse-grained potential. By design it appropriately predicts zero mixing due to local interparticle interactions. For example, it predicts that the chaotic mixing time is infinite for linear external and space-charge forces. In this limit the particle density is uniform, and one can see from Eqs. (9) and (11) that the corresponding Lyapunov exponent is zero. The same can be seen, of course, in the case that the external forces are linear and there is no space charge, *i.e.*, $\omega_p = 0$.

With the aid of a more general metric, specifically a Finsler metric, the geometrodynamic method can be generalized to include a potential that is both time-dependent and velocity-dependent.[17] It is therefore potentially applicable to a wide variety of beam-dynamics problems. For example, one might be able to develop a geometric measure of chaos over a Finsler manifold for use in rapidly constructing a system's Poincaré surface of section, as has been done for the Hénon-Heiles potential.[18] If so, then the method may provide an efficient means of calculating dynamic apertures in circular machines in which magnet nonlinearities, and perhaps beam-beam interactions, establish parametric resonances that gradually degrade the beam. Traditional methods require very long integration times and their attendant numerical difficulties.

In the case of a beam under the influence of a time-dependent potential, one can postulate a lowest-order approximation in which the principal effect of the time dependence on chaotic mixing is to establish various parametric resonances. These could arise, for example, by way of resonant coupling between space-charge modes and a periodic transport lattice. The mixing time would then follow from the methodology presented here, wherein the time-averaged potential forms the basis for defining the microcanonical ensemble. The result takes the form of Eq. (11), and insofar as it involves the depressed betatron frequency via the ratio ω_s/ω_{po}, it agrees with "relaxation" time scales observed in simulations and experiments.[13] However, one must take care not to infer too much from this conjecture. The Eisenhart metric, being independent of velocity space, cannot account for energy exchange between space-charge modes and individual particles. Thus, important processes such as violent relaxation and attendant halo formation are missing.[19,20] In principle, they can be accessed with a Finsler metric.

As a final remark, it will be of interest to compare the geometrodynamic predictions against numerical experiments specifically focussed on the behavior of particle trajectories and their associated mixing in the presence of nonlinear space-charge forces. In this context the evolution of particle ensembles that could represent, for example, initially localized perturbations ostensibly caused by transient forces external to the bunch is of special interest.

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