

# Space Charge Effects in Real and Simulated Charged Particle Beams Review of the Understanding of PIC Noise

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- **Review on statistical mechanics: Langevin equation**
- Fokker-Planck equation
- Moment analysis of the Fokker-Planck equation
- Generalized beam envelope equations
- Emittance growth rates
- Numerical examples
- Irreversibility in computer simulations
- Summary

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# Review on Statistical Mechanics: Langevin Equation

Space Charge effects including intra-beam scattering: multiple small-angle Coulomb scattering within a charged particle beam that circulates in a storage ring.

↪ basically  $N$ -body problem with  $N$  very large, fully determined by both the coupled single particle equations of motion

$$m \frac{d^2 \mathbf{x}_i}{dt^2} - \mathbf{F}_{\text{ext}}(\mathbf{x}_i, t) - \frac{q^2}{4\pi\epsilon_0} \sum_{j \neq i} \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3} = 0, \quad i = 1, \dots, N$$

and the initial  $N$ -body distribution function

$$\rho(\mathbf{x}, \mathbf{v}, t_0) = \sum_i \delta^3(\mathbf{x} - \mathbf{x}_i(t_0)) \delta^3(\mathbf{v} - \mathbf{v}_i(t_0))$$

↪ the granular nature of the beam's charge distribution must be taken into account

↪ for analytical approaches, only a statistical description is possible

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A statistical description means to replace the exact, fine-grained Coulomb force  $\mathbf{E}_{\text{sc}}$  by its smoothed, continuous average force

$$\mathbf{E}_{\text{sc}}(\mathbf{x}, t) \longrightarrow \mathbf{E}_{\text{sc}}^{\text{sm}}(\mathbf{x}, t)$$

The fine-grained aspect of the particle motion is then modeled by an additional fluctuating force  $\mathbf{F}_{\text{L}}(\mathbf{x}, t)$  that has only statistically defined properties. This force must vanish on the average over all particles

$$\langle \mathbf{F}_{\text{L}} \rangle = 0$$

Furthermore, a force referred to as **dynamical friction**  $\mathbf{F}_{\text{fr}}(\mathbf{v}, t)$  must be introduced to obtain the statistical counterpart of the deterministic single particle equation of motion, referred to as the **Langevin equation**

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The amplitudes of  $\mathbf{F}_{\text{fr}}$  and  $\mathbf{F}_{\text{L}}$  depend on each other  
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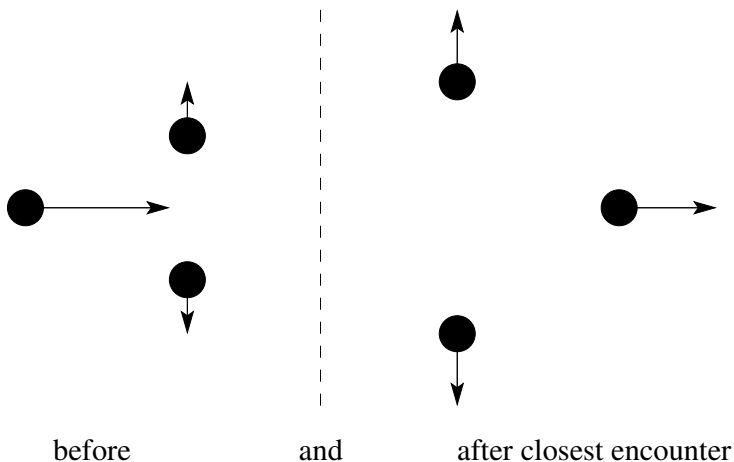
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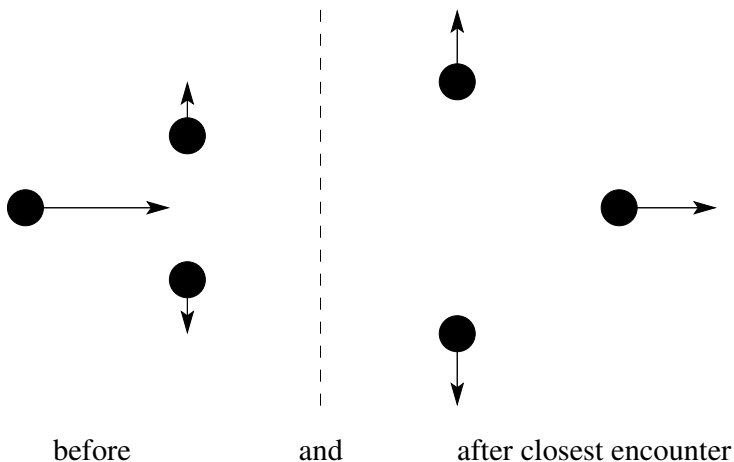


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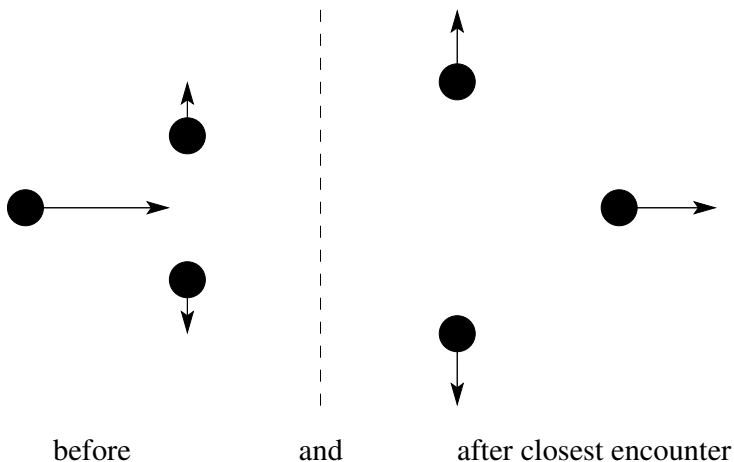
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# Fokker-Planck Equation

A formal solution of the Langevin equation is not possible.

Instead, on the basis of the Langevin equation, we can set up the Fokker-Planck equation in order to determine the time evolution of the **probability density**  $f$ , defined as the 6-dimensional “ $\mu$ -phase-space” density function

$$f = f(\mathbf{x}, \mathbf{v}, t)$$

- $f \, d\mathbf{x} \, d\mathbf{v}$  provides the probability finding a particle inside the volume  $d\mathbf{x} \, d\mathbf{v}$  around the phase-space point  $\mathbf{q} \equiv (\mathbf{x}, \mathbf{v})$  at time  $t$ .
- $f$  is a smooth function of the phase-space variable  $\mathbf{q}$ .

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Fokker-Planck equation: Replacement of the **reversible** original problem of solving  $N$  coupled second order differential equations by **one** equation of motion for the probability density  $f$ :

$$\frac{\partial f}{\partial t} = \mathbf{L}_{\text{FP}} f$$

- ↪ We have given up the knowledge on the location of individual particles.
- ↪ We restrict ourselves to the knowledge of the evolution of the probability density function  $f$ .
- ↪ The phenomenon of **irreversibility** emerges as a result of this description (to be discussed later in this talk).

With the particular Langevin equation from above

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the Fokker-Planck operator  $\mathbf{L}_{\text{FP}}$  reduces to

$$\mathbf{L}_{\text{FP}} = \sum_{i=1}^3 \left[ -\frac{\partial}{\partial \mathbf{x}_i} v_i - \frac{1}{m} \frac{\partial}{\partial v_i} F_{\text{tot},i} + \frac{\partial^2}{\partial v_i^2} D_{ii} \right],$$

with  $F_{\text{tot},i}$  defined as the sum of all **non-Langevin forces**

$$F_{\text{tot},i}(\mathbf{x}, \mathbf{v}, t) = F_{\text{ext},i}(\mathbf{x}, t) + qE_{\text{sc},i}^{\text{sm}}(\mathbf{x}, t) + F_{\text{fr},i}(v_i, t),$$

and the diffusion coefficients  $D_{ij}$

$$\langle F_{L,i}(v_i, t) F_{L,j}(v_j, t') \rangle = 2m^2 D_{ij}(v_i, t) \delta_{ij} \delta(t - t').$$

- The FP equation describes a diffusion process in velocity space that is counteracted by the dynamical friction.
- The process evolves within an effective potential given by the external focusing and the smooth part of the self-fields.
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# Discussion of the Fluctuation-Dissipation Theorem

Systems in dynamical equilibrium are governed by

- **diffusion: effect that drives a quantity off its steady-state value (fluctuation)**
- friction: effect that causes the decay of this deviation from the steady-state value (dissipation)

The diffusion process and friction effects are **not independent** of each other.

↪ Both effects are related by a fluctuation-dissipation theorem

↪ Simplest case (isotropic process): Einstein relation

$$D \equiv D_{ij} = \beta_f \frac{k_B T_{\text{eq}}}{m}.$$

We will use this simple approximation in our approach.

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# Moment Analysis of the Fokker-Planck Equation

A direct solution of the Fokker-Planck equation would

- be too costly
- yield too much information since the detailed knowledge of  $f$  is not necessary in order to estimate stochastic effects in ion beams

A usual way to switch to more global physical quantities is to consider moments of  $f(\mathbf{x}, \mathbf{v}, t)$ :

$$\langle x^2 \rangle(t) = \int x^2 f d\tau, \quad d\tau = d^3x_i d^3v_i$$

$\sqrt{\langle x^2 \rangle}$  is proportional to the actual beam width in  $x$ .

The derivatives of the moments are calculated according to

$$\frac{d}{dt} \langle x^2 \rangle = \int x^2 \frac{\partial f}{\partial t} d\tau,$$

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and inserting  $\partial f / \partial t = \mathbf{L}_{\text{FP}} f$ .

# Moment Analysis of the Fokker-Planck Equation

A direct solution of the Fokker-Planck equation would

- be too costly
- yield too much information since the detailed knowledge of  $f$  is not necessary in order to estimate stochastic effects in ion beams

A usual way to switch to more **global** physical quantities is to consider **moments of  $f(\mathbf{x}, \mathbf{v}, t)$** :

$$\langle x^2 \rangle(t) = \int x^2 f d\tau, \quad d\tau = d^3x_i d^3v_i$$

$\sqrt{\langle x^2 \rangle}$  is proportional to the actual beam width in  $x$ .

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Integrating by parts, we obtain for each phase-space plane  $i$  a coupled set of **moment equations**

$$\frac{d}{dt} \langle x_i^2 \rangle - 2 \langle x_i v_i \rangle = 0$$

$$m \frac{d}{dt} \langle x_i v_i \rangle - m \langle v_i^2 \rangle - \langle x_i F_{\text{ext},i} \rangle - q \langle x_i E_{\text{sc},i}^{\text{sm}} \rangle = \langle x_i F_{\text{fr},i} \rangle$$

$$m \frac{d}{dt} \langle v_i^2 \rangle - 2 \langle v_i F_{\text{ext},i} \rangle - 2q \langle v_i E_{\text{sc},i}^{\text{sm}} \rangle = 2 \langle v_i F_{\text{fr},i} \rangle + 2m \langle D_{ii} \rangle$$

As usual, we define the rms emittance  $\varepsilon_i(t)$  as

$$\varepsilon_i^2(t) = \langle x_i^2 \rangle \langle v_i^2 \rangle - \langle x_i v_i \rangle^2$$

The time derivative of the rms emittance may be arranged as

$$\frac{d}{dt} \varepsilon_i^2(t) = \left. \frac{d}{dt} \varepsilon_i^2(t) \right|_{\text{ext}} + \left. \frac{d}{dt} \varepsilon_i^2(t) \right|_{\text{sc}} + \left. \frac{d}{dt} \varepsilon_i^2(t) \right|_{\text{ir}}$$

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$\left. \frac{d}{dt} \varepsilon_i^2(t) \right|_{\text{ext}}$  and  $\left. \frac{d}{dt} \varepsilon_i^2(t) \right|_{\text{sc}}$  describe the **reversible** emittance change effects due to non-linear external focusing forces and non-linear electric self-fields.

$$\begin{aligned} \left. \frac{m}{2} \frac{d}{dt} \varepsilon_i^2(t) \right|_{\text{ext}} &= \langle x_i^2 \rangle \langle v_i F_{\text{ext},i} \rangle - \langle x_i v_i \rangle \langle x_i F_{\text{ext},i} \rangle \\ &= 0 \quad \iff \quad F_{\text{ext},i} \propto x_i. \end{aligned}$$

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# Generalized Beam Envelope Equations

With

$$F_{\text{fr},i} = -m\beta_f v_i, \quad F_{\text{ext},i} = -m\omega_i^2(t) x_i$$

we obtain the well-known envelope equation from the first two moment equations with an **additional** damping term

$$\frac{d^2}{dt^2} \sqrt{\langle x_i^2 \rangle} + \beta_f \frac{d}{dt} \sqrt{\langle x_i^2 \rangle} + \omega_i^2(t) \sqrt{\langle x_i^2 \rangle} - \frac{q}{m} \frac{\langle x_i E_{\text{sc},i}^{\text{sm}} \rangle}{\sqrt{\langle x_i^2 \rangle}} - \frac{\varepsilon_i^2(t)}{\sqrt{\langle x_i^2 \rangle}^3} = 0$$

For the irreversible emittance change, the above approximations lead to

$$\left. \frac{1}{\langle x_i^2 \rangle} \frac{d}{dt} \varepsilon_i^2(t) \right|_{\text{ir}} = 2\beta_f \left( \frac{k_B T_{\text{eq}}}{m} - \frac{\varepsilon_i^2(t)}{\langle x_i^2 \rangle} \right)$$

→ Simple temperature relaxation equation

→ Closed set of differential equations for  $\sqrt{\langle x_i^2 \rangle}$  and  $\varepsilon_i^2(t)$ .





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# Non-Equilibrium Beam Temperatures

For charged particle beams, we define the generalized, **non-equilibrium temperature**  $k_B T_i$  as the **incoherent part of the kinetic energy** of the beam particles in the  $i$ -th degree of freedom:

$$k_B T_i \equiv m \left\langle (v_i^{\text{inc}})^2 \right\rangle, \quad v_i^{\text{inc}} = v_i - x_i \frac{\langle x_i v_i \rangle}{\langle x_i^2 \rangle}$$

since the total kinetic energy  $m \langle v_i^2 \rangle / 2$  contains a coherent part if  $\langle x_i v_i \rangle \neq 0$ . With the rms emittance  $\varepsilon_i$  defined by

$$\varepsilon_i^2(t) = \langle x_i^2 \rangle \langle v_i^2 \rangle - \langle x_i v_i \rangle^2,$$

the non-equilibrium temperature  $k_B T_i$  of the  $i$ -th degree of freedom can then be expressed as

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# Equilibrium Temperature

With  $k_B T_{z,b} = m \langle (\Delta v_{z,b})^2 \rangle$ , the longitudinal temperature in the beam frame, we may define the equilibrium temperature  $T_{\text{eq}}$  as the **arithmetic mean** of the temperatures  $T_x$ ,  $T_y$ , and  $T_z$

$$\frac{k_B T_{\text{eq}}}{m} = \frac{k_B}{3m} (T_x + T_y + T_z) = \frac{1}{3} \left( \frac{\epsilon_x^2}{\langle x^2 \rangle} + \frac{\epsilon_y^2}{\langle y^2 \rangle} + \langle (\Delta v_{z,b})^2 \rangle \right)$$

For a coasting beam in a strong focusing system, we have

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# Emittance Growth Rates

With the temperature relations, the above formula for the irreversible emittance growth is obtained for the x-direction as

$$\frac{1}{\langle x^2 \rangle} \frac{d}{dt} \varepsilon_x^2(t) \Big|_{\text{ir}} = -\frac{2\beta_f}{3} \left( \frac{2\varepsilon_x^2(t)}{\langle x^2 \rangle} - \frac{\varepsilon_y^2(t)}{\langle y^2 \rangle} - \langle (\Delta v_{z,b})^2 \rangle \right),$$

or, equivalently, with the **temperature ratios**

$$r_{xy} = \frac{T_y(t)}{T_x(t)}, \quad r_{xz} = \frac{T_z(t)}{T_x(t)}, \quad r_{yz} = \frac{T_z(t)}{T_y(t)}$$

as

$$\frac{d}{dt} \ln \varepsilon_x^2(t) \Big|_{\text{ir}} = \frac{2\beta_f}{3} (r_{xy} + r_{xz} - 2).$$

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# Entropy

Summing over all three degrees of freedom, we get

$$\frac{1}{k_B} \frac{dS}{dt} \stackrel{\text{Def}}{=} \frac{d}{dt} \ln \varepsilon_x^2 \varepsilon_y^2 \varepsilon_z^2 \Big|_{\text{ir}} = \frac{2\beta_f}{3} \left( \frac{(1 - r_{xy})^2}{r_{xy}} + \frac{(1 - r_{xz})^2}{r_{xz}} + \frac{(1 - r_{yz})^2}{r_{yz}} \right) \geq 0.$$

- The change of the "total emittance" is always positive
- $S$  has the character of an **entropy** within a closed system

Integration yields the  $e$ -folding time  $\tau_{\text{ef}}$  of the total emittance  $\varepsilon$

$$\tau_{\text{ef}}^{-1} = \frac{1}{9} \beta_f (I_{xy} + I_{xz} + I_{yz}), \quad \varepsilon = \sqrt[3]{\varepsilon_x \varepsilon_y \varepsilon_z}$$

with the **local temperature imbalance integrals** per period (turn)  $T$

$$I_{xy} = \frac{1}{T} \int_0^T \frac{[1 - r_{xy}(t)]^2}{r_{xy}(t)} dt \geq 0, \quad r_{xy}(t) = \frac{\varepsilon_y^2}{\langle y^2 \rangle} \frac{\langle x^2 \rangle}{\varepsilon_x^2}.$$

We will see that this description also applies to **computer noise** effects in simulations of charged particle beams.

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With the abbreviations

$$a = \sqrt{\langle x^2 \rangle}$$

$$b = \sqrt{\langle y^2 \rangle}$$

$$\delta = \sqrt{\langle (\Delta p/p)^2 \rangle}$$

$$D = \Delta x / (\Delta p/p)$$

$$\eta = \gamma^{-2} - D/\rho$$

$$A = \sqrt{a^2 + D^2 \delta^2}$$

$$K = 2Ze_0 I / (4\pi\epsilon_0 mc^3 \beta^3 \gamma^3)$$

the complete system of moment equations for a coasting beam with elliptic cross section in real space and generalized perveance  $K$  that propagates through a dispersive system reads:



# Complete Closed Set of Moment Equations

$$\ddot{a} + \beta_f \dot{a} + \omega_x^2 a - \frac{K/2}{A(A+b)} a - \frac{\varepsilon_x^2}{a^3} = 0$$

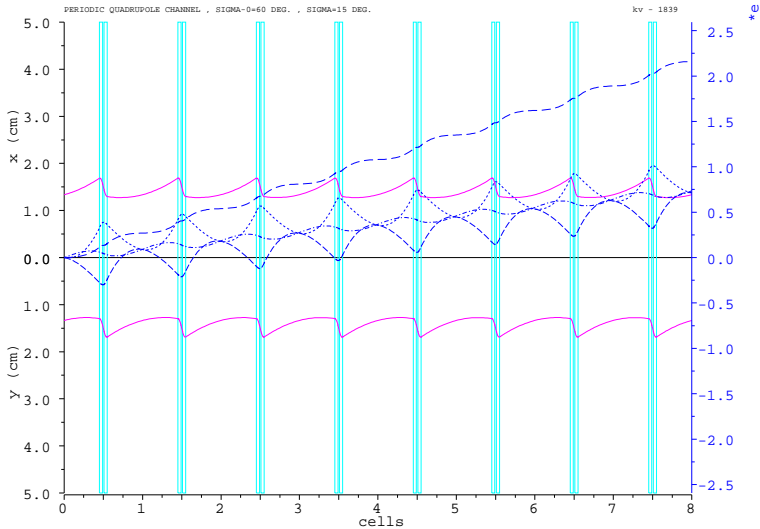
$$\ddot{b} + \beta_f \dot{b} + \omega_y^2 b - \frac{K/2}{A+b} - \frac{\varepsilon_y^2}{b^3} = 0$$

$$\ddot{D} + (\omega_x^2 - \rho^{-2}) D - \frac{K/2}{A(A+b)} D - \frac{1}{\rho} = 0$$

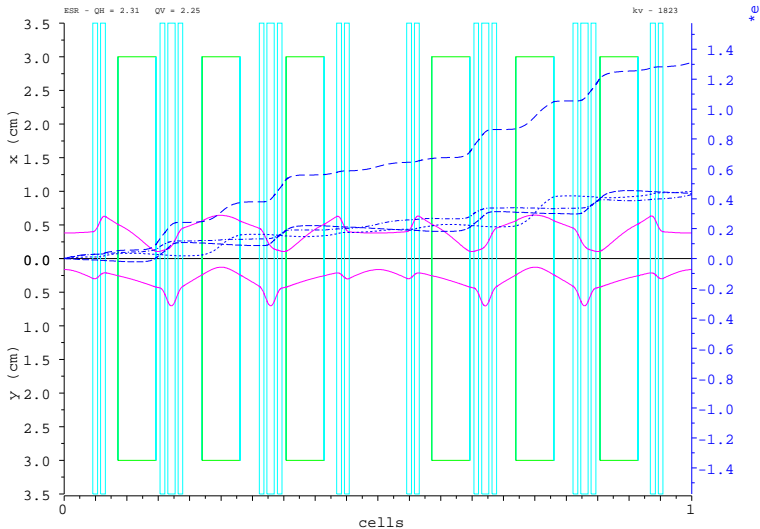
$$\frac{1}{a^2} \frac{d}{dt} \varepsilon_x^2 + \frac{2}{3} \beta_f \left( 2 \frac{\varepsilon_x^2}{a^2} - \frac{\varepsilon_y^2}{b^2} - \eta \delta^2 \right) = 0$$

$$\frac{1}{b^2} \frac{d}{dt} \varepsilon_y^2 + \frac{2}{3} \beta_f \left( 2 \frac{\varepsilon_y^2}{b^2} - \frac{\varepsilon_x^2}{a^2} - \eta \delta^2 \right) = 0$$

$$\eta \frac{d}{dt} \delta^2 + \frac{2}{3} \beta_f \left( 2 \eta \delta^2 - \frac{\varepsilon_x^2}{a^2} - \frac{\varepsilon_y^2}{b^2} \right) = 0$$



Beam envelopes (red lines) and emittance and momentum spread growth factors (dashed lines) in a FODO channel. The scale on the right hand side applies to the emittance growth functions.



Beam envelopes (solid lines) and emittance and momentum spread growth factors (dashed lines) along one turn in the GSI Experimental Storage Ring (ESR).

# Irreversibility in Computer Simulations

The friction forces  $F_{\text{fr},i}$  must always be decelerating.

$$F_{\text{fr},i}(v_i) = -F_{\text{fr},i}(-v_i), \quad \rightsquigarrow D_{ii}(v_i) = D_{ii}(-v_i).$$

Transformation that reverses the direction of time flow:

$$t \rightarrow -t \quad \rightsquigarrow x_j \rightarrow x_j, \quad v_j \rightarrow -v_j.$$

We may separate the components of the Fokker-Planck operator with respect to their behavior under time reversal

$$\mathcal{L}_{\text{FP}} = \mathcal{L}_{\text{rev}} + \mathcal{L}_{\text{ir}}.$$

The reversible operator  $\mathcal{L}_{\text{rev}}$ : terms that change sign under time reversal, hence leave  $\partial f / \partial t = \mathcal{L}_{\text{rev}} f$  invariant.

$\rightsquigarrow$  Earlier states are fully restored — just like a movie that is reversed at some instant of time  $t_0$   $\rightsquigarrow$  Vlasov equation.

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The smooth self-field  $\mathbf{E}_{\text{sc}}^{\text{sm}}$  is obtained from the real space projection of the probability density  $f(\mathbf{q}, t)$  via Poisson's equation.

The components that do not change sign make up  $\mathbf{L}_{\text{ir}}$

$$\mathbf{L}_{\text{ir}} = \sum_{i=1}^3 \frac{\partial}{\partial v_i} \left[ -\frac{F_{\text{fr},i}(v_i, t)}{m} + \frac{\partial}{\partial v_i} D_{ii}(v_i, t) \right].$$

$\mathbf{L}_{\text{ir}}$  describes those effects that do *not* depend on the direction of the time flow. In other words, it describes the **irreversible** aspects of the particle motion.

Real system: mixture of reversible and irreversible behavior.



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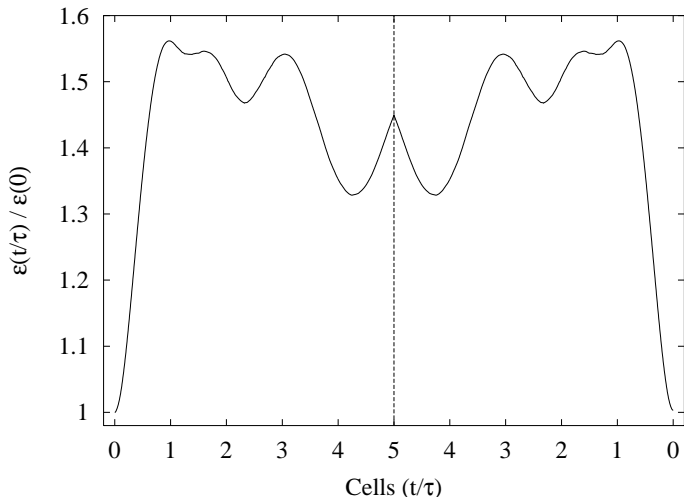
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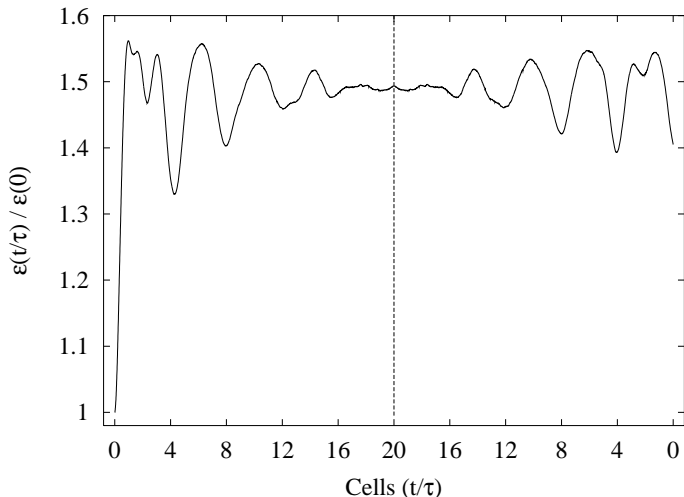
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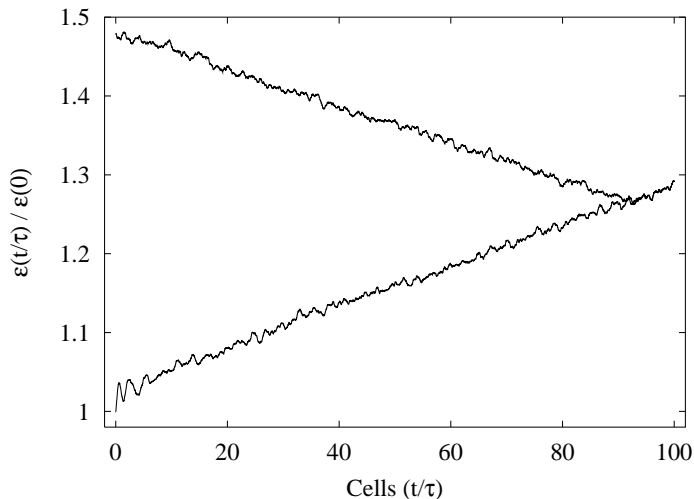
Emittance growth factors versus number of cells obtained for a non-stationary initial phase-space density at  $\sigma_0 = 60^\circ$ ,  $\sigma = 15^\circ$ , 2500 simulation particles.

The vertical dashed line marks the point of time reversal after 5 cells.

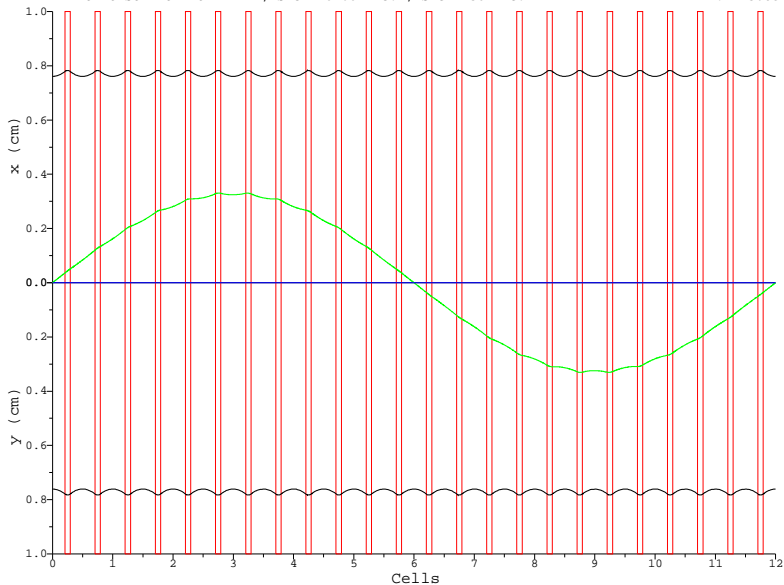


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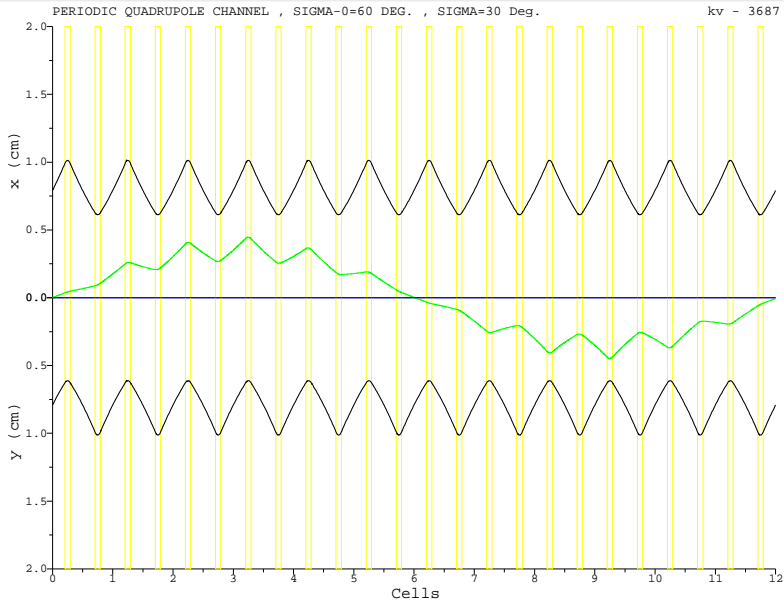
The vertical dashed line marks the point of time reversal after 20 cells.



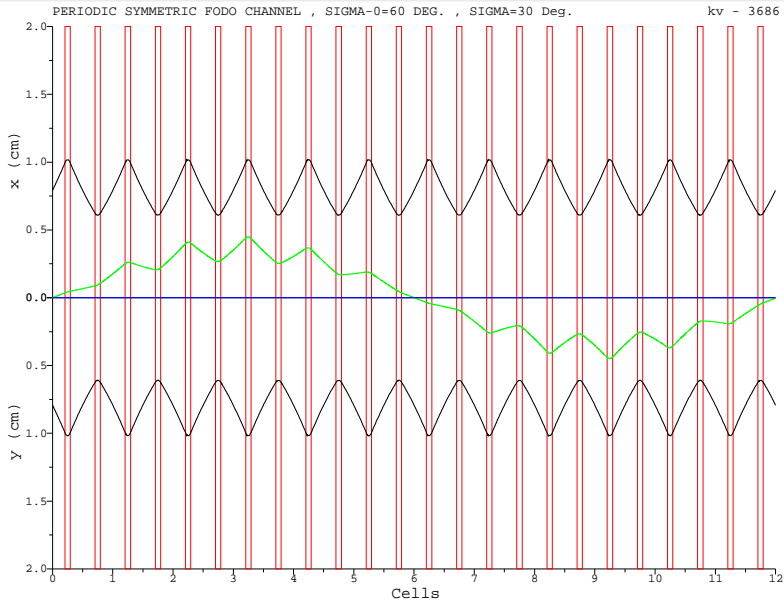
Emittance growth factors versus number of cells obtained by 3-D simulations of a periodic non-isotropic focusing system at  $\sigma_0 = 60^\circ$ ,  $\sigma = 15^\circ$  per cell, 2000 simulation particles. After 100 cells the time reversal occurs.



Periodic solenoid channel (FOFO),  $\sigma_0 = 60^\circ$ ,  $\sigma = 30^\circ$ .



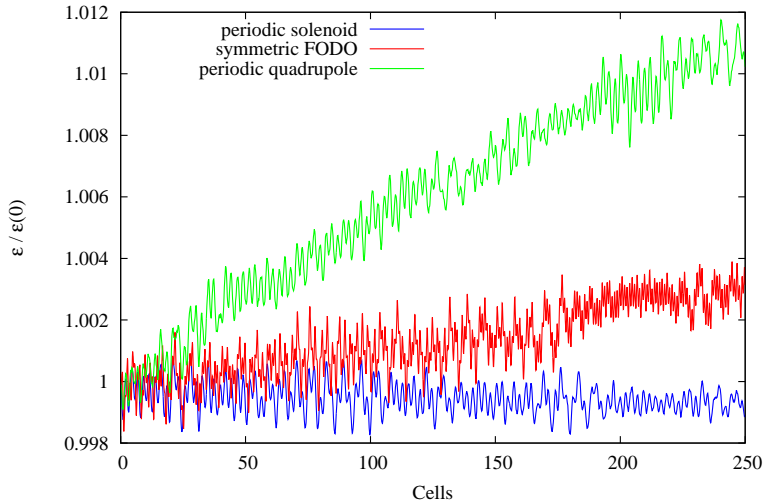
Periodic quadrupole channel (FODO),  $\sigma_0 = 60^\circ$ ,  $\sigma = 30^\circ$ .



Fictitious symmetric FODO channel,  $\sigma_0 = 60^\circ$ ,  $\sigma = 30^\circ$ .

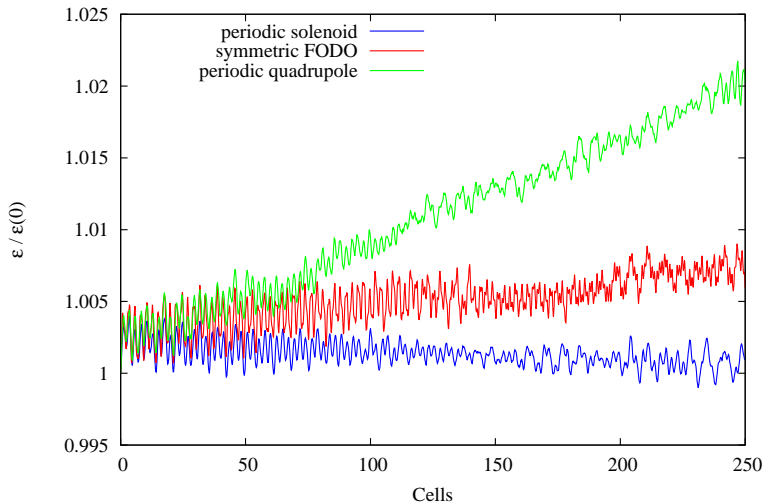


Periodic transport channels,  $\sigma_0=60^\circ$ ,  $\sigma=30^\circ$ , 10000 particles, Poisson solver



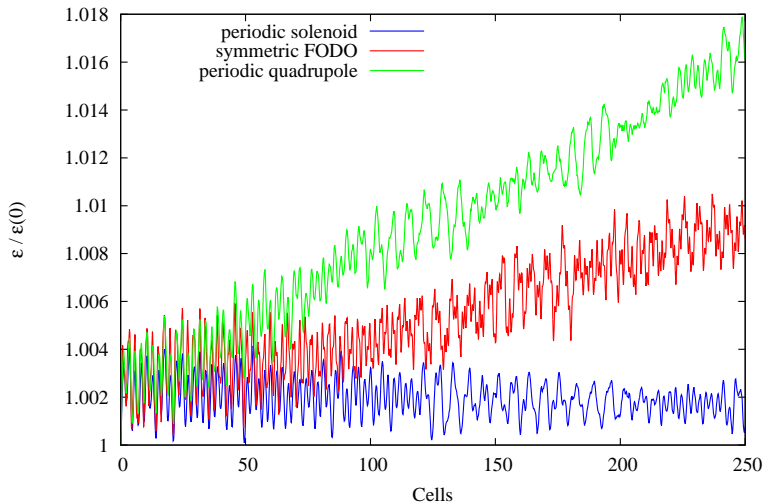
2D emittance growth factors versus number of cells for different focusing lattices,  $10^4$  simulation particles, and 256 mesh points.

Periodic transport channels,  $\sigma_0=60^\circ$ ,  $\sigma=30^\circ$ , 5000 particles, Poisson solver



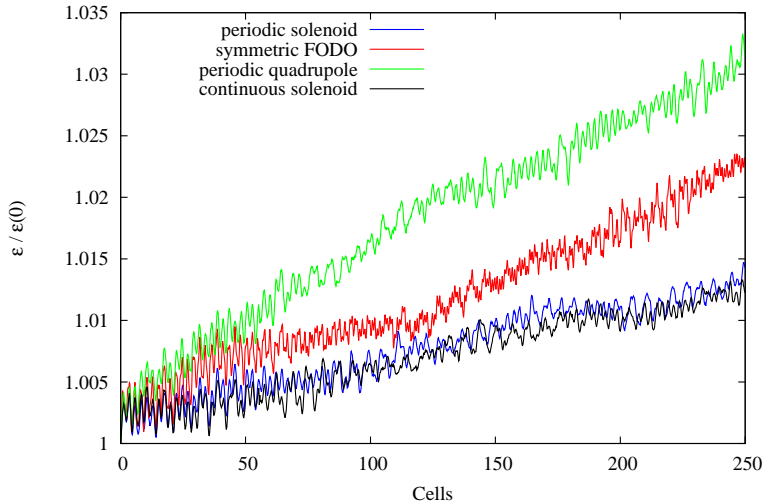
2D emittance growth factors versus number of cells for different focusing lattices,  $5 \cdot 10^3$  simulation particles, and 256 mesh points.

Periodic transport channels,  $\sigma_0=60^\circ$ ,  $\sigma=30^\circ$ , 5000 particles, Poisson solver



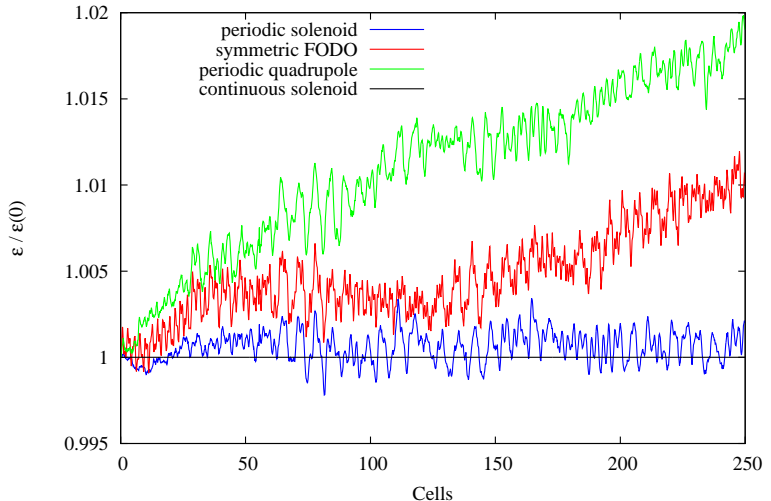
2D emittance growth factors versus number of cells for different focusing lattices,  $5 \cdot 10^3$  simulation particles, and 128 mesh points.

Periodic focusing channels,  $\sigma_0=60^\circ$ ,  $\sigma=30^\circ$ , 5000 particles, p-p-int



2D emittance growth factors versus number of cells for different focusing lattices,  $5 \cdot 10^3$  simulation particles, and particle-particle interaction.

Periodic focusing channels,  $\sigma_0=60^\circ$ ,  $\sigma=30^\circ$ , 5000 particles, p-p-int, norm.



Normalized 2D emittance growth factors versus number of cells for different focusing lattices,  $5 \cdot 10^3$  simulation particles, and particle-particle interaction.

# Summary

- The Fokker-Planck equation provides the starting point for analytical approaches in the physics of charged particle beams if the actual charge granularity cannot be neglected.
- The moment analysis of the Fokker-Planck equation consistently extends F. Sacherer's moment analysis of the Vlasov equation.
- As a good approximation, the emittance growth rates that are due to intra-beam scattering depend on both the accumulated temperature imbalances along a storage ring and the friction coefficient  $\beta_f$ , which represents the only characteristic parameter of the statistical description.
- The approach also applies for the description of noise effects in computer simulations.
- In that case, the parameter  $\beta_f$  measures the deviation from a completely reversible numerical calculation ( $\beta_f = 0$ ).

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