Stochastic Effects in Real and Simulated Charged Particle Beams

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Outline

- Review on statistical mechanics: Langevin equation
- Fokker-Planck equation
- Fixing of the Fokker-Planck coefficients for intra-beam scattering (IBS)
- Moment analysis of the Fokker-Planck equation
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- Emittance growth rates
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Review on Statistical Mechanics: Langevin Equation

Intrabeam 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

\[ m \frac{d^2 x_i}{dt^2} - F_{\text{ext}}(x_i, t) - \frac{q^2}{4\pi\epsilon_0} \sum_{j \neq i} \frac{x_i - x_j}{|x_i - x_j|^3} = 0, \quad i = 1, \ldots, N \]

and the initial N-body distribution function

\[ \rho(x, v, t_0) = \sum_i \delta^3(x - x_i(t_0)) \delta^3(v - v_i(t_0)) \]

~~ the granular nature of the beam’s charge distribution must be taken into account

~~ for analytical approaches, only a statistical description is possible

A statistical description means to replace the exact, fine-grained Coulomb force \( E_{\text{sc}} \) by its smoothed, continuous average force

\[ E_{\text{sc}}(x, t) \rightarrow E_{\text{sc}}^{\text{sm}}(x, t) \]

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

\[ \langle F_L \rangle = 0 \]

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

\[ m \frac{d^2 x}{dt^2} - F_{\text{ext}} - qE_{\text{sc}}^{\text{sm}} - F_{\text{fr}} = F_L. \]

The amplitudes of \( F_{\text{fr}} \) and \( F_L \) depend on each other

~~ fluctuation-dissipation theorem
The effect of dynamical friction for repelling forces may be visualized as before and after closest encounter.

As is easily verified, a friction also occurs for attracting forces.

The general form of the Langevin equation can be written as

\[ \dot{q}_i = K_i(q, t) + \Gamma_i(q, t), \quad i = 1, \ldots, 6, \]

with smooth functions \( K_i(q, t) \). For the random variables, one assumes the \( \Gamma_i(q, t) \) to be Gaussian-distributed and

\[ \langle \Gamma_i(q, t) \rangle = 0, \quad \langle \Gamma_i(q, t) \Gamma_j(q, t') \rangle = 2Q_{ij}(q, t) \delta(t - t'). \]

Under these conditions, the Kramers expansion for \( \partial f(q, t)/\partial t \) terminates after the second term. The expansion with only the first and second term is called Fokker-Planck equation

\[ \frac{\partial f}{\partial t} = L_{\text{FP}} f \]

with the Fokker-Planck operator \( L_{\text{FP}} \) given by

\[ L_{\text{FP}} = -\sum_{i=1}^{6} \frac{\partial}{\partial q_i} K_i(q, t) + \sum_{i,j=1}^{6} \frac{\partial^2}{\partial q_i \partial q_j} Q_{ij}(q, t) \]

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

\[ f = f(x, v, t) \]

\[ \rightarrow f \, dx \, dv \] provides the probability finding a particle inside the volume \( dx \, dv \) around the phase-space point \( q \equiv (x, v) \) at time \( t \).

\[ \rightarrow f \] is a smooth function of the phase-space variable \( q \).

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 \( f \):

\[ \frac{\partial f}{\partial t} = L_{\text{FP}} f \]

\[ \rightarrow \] We have given up the knowledge on the location of individual particles.

\[ \rightarrow \] We restrict ourselves to the knowledge of the evolution of the probability density function \( f \).

\[ \rightarrow \] 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

\[ m \frac{d^2x}{dt^2} = F_{\text{ext}} + qE_{\text{sc}}^\text{m} + F_{\text{fr}} + F_L \]
The Fokker-Planck operator $L_{FP}$ reduces to

$$L_{FP} = \sum_{i=1}^{3} \left[ -\frac{\partial}{\partial x_i} v_i - \frac{1}{m} \frac{\partial}{\partial v_i} F_{tot,i} + \frac{\partial^2}{\partial v_i^2} D_{ii} \right],$$

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

$$F_{tot,i}(x, v, t) = F_{ext,i}(x, t) + qE_{sm,i}(x, t) + F_{fr,i}(v_i, t),$$

and the diffusion coefficients $D_{ii}$

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

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.

The Langevin forces occurring in the given system may be any kind of random forces of physical or numerical nature.

The Coulomb logarithm $\ln \Lambda$ is generally given by

$$\ln \Lambda \approx \ln \frac{b_m}{b_\perp},$$

with

- $b_m$ the maximum value of the impact parameter,
- $b_\perp$ the impact parameter corresponding to a 90° deflection.

For non-neutralized systems $b_m$ is set to the average distance between the particles (“ion sphere radius”). This yields

$$\Lambda \approx \frac{3k_B T_{eq}}{2Z^2 r_c mc^2 n^{1/3}},$$

with $n$ the particle density and $T_{eq}$ the equilibrium temperature. We summarize

- fixing $\beta_f$ is the major source of inaccuracy
- plasma physics reasoning, hence common to all approaches on intra-beam scattering

Fixing of the Fokker-Planck Coefficients for IBS

For the effect of intra-beam scattering, $F_{fr,i}$ can be obtained by

- solving the equations of motion for a single small angle scattering event
- averaging over all allowable impact parameters,
- subsequently averaging over the particle velocity distribution.

“Not too far” from thermodynamic equilibrium, $F_{fr,i}$ is given by

$$F_{fr,i} = -m\beta_f v_i, \quad \beta_f = \frac{1}{\sqrt{2\pi \beta^3} \frac{Z^4}{A^2} \cdot r_c^2 \cdot N \frac{\epsilon_x \epsilon_y \epsilon_z}{\ln \Lambda}} \ln \Lambda,$$

with $r_c = \frac{e^2}{4\pi\epsilon_0 mc^2}$ the classical particle radius, and $Z$ and $A$ the charge and mass numbers of the $N$-particle ensemble. $\epsilon_i$ denotes the emittance in the $i$-th phase-space plane.

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

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

We will use this simple approximation in our approach.
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 \( f \):

\[
\langle x^2 \rangle = \int x^2 f \, \mathrm{d}x
\]

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

The derivatives of the moments are calculated according to

\[
\frac{\mathrm{d}}{\mathrm{d}t} \langle x^2 \rangle = \int x^2 \frac{\partial f}{\partial t} \, \mathrm{d}x,
\]

and inserting \( \frac{\partial f}{\partial t} = L_{FP} f \).

\[
\frac{\mathrm{d}}{\mathrm{d}t} \varepsilon_i^2(t)\bigg|_{\text{ext}} \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t} \varepsilon_i^2(t)\bigg|_{\text{sc}} \quad \text{describe the reversible emittance change effects due to non-linear external focusing forces and non-linear electric self-fields.}
\]

\[
\frac{m}{2} \frac{\mathrm{d}}{\mathrm{d}t} \varepsilon_i^2(t)\bigg|_{\text{ext}} = \langle x_i^2 \rangle \langle v_i F_{\text{ext},i} \rangle - \langle x_i v_i \rangle \langle x_i F_{\text{ext},i} \rangle
\]

\[
= 0 \quad \iff \quad F_{\text{ext},i} \propto x_i.
\]

\[
\frac{m}{2} \frac{\mathrm{d}}{\mathrm{d}t} \varepsilon_i^2(t)\bigg|_{\text{sc}} = q \left[ \langle x_i^2 \rangle \langle v_i E_{\text{sc},i}^\text{em} \rangle - \langle x_i v_i \rangle \langle x_i E_{\text{sc},i}^\text{em} \rangle \right].
\]

The third contribution to the change of the emittance emerges from the irreversible Fokker-Planck operator \( L_i \).

\[
\frac{m}{2} \frac{\mathrm{d}}{\mathrm{d}t} \varepsilon_i^2(t)\bigg|_{\text{ir}} = \langle x_i^2 \rangle \langle v_i F_{\text{ir},i} \rangle - \langle x_i v_i \rangle \langle x_i F_{\text{ir},i} \rangle + m \langle x_i^2 \rangle \langle D_i \rangle.
\]

\( \Rightarrow \) The rms emittance growth depends on both the Fokker-Planck coefficients and and the specific shape of the envelope functions.

\[
\frac{\mathrm{d}}{\mathrm{d}t} \langle x_i^2 \rangle - 2 \langle x_i v_i \rangle = 0
\]

\[
m \frac{\mathrm{d}}{\mathrm{d}t} \langle x_i v_i \rangle - m \langle v_i^2 \rangle - \langle x_i F_{\text{ext},i} \rangle - q \langle x_i E_{\text{sc},i}^\text{em} \rangle = \langle x_i F_{\text{ir},i} \rangle
\]

\[
m \frac{\mathrm{d}}{\mathrm{d}t} \langle v_i^2 \rangle - 2 \langle v_i F_{\text{ext},i} \rangle - 2 q \langle v_i E_{\text{sc},i}^\text{em} \rangle = 2 \langle v_i F_{\text{ir},i} \rangle + 2 m \langle D_i \rangle
\]

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

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

Generalized Beam Envelope Equations

With

\[
F_{\text{ir},i} = -m \beta_i v_i, \quad F_{\text{ext},i} = -m \omega_i^2(t) x_i
\]

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

\[
\frac{d^2}{dt^2} \sqrt{\langle x_i^2 \rangle} + \beta_i \frac{d}{dt} \sqrt{\langle x_i^2 \rangle} + \omega_i^2(t) \sqrt{\langle x_i^2 \rangle} - \frac{q}{m} \frac{\langle x_i E_{\text{sc},i}^\text{em} \rangle}{\sqrt{\langle x_i^2 \rangle}} - \frac{\varepsilon_i^2(t)}{\sqrt{\langle x_i^2 \rangle}} = 0
\]

For the irreversible emittance change, the above approximations lead to

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

\( \Rightarrow \) Simple temperature relaxation equation

\( \Rightarrow \) Closed set of differential equations for \( \sqrt{\langle x_i^2 \rangle} \) and \( \varepsilon_i^2(t) \).
With the rms emittance $\varepsilon_i$, 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:

$$k_B T_i = m \langle \langle v_{i}^{\text{inc}} \rangle^2 \rangle, \quad v_{i}^{\text{inc}} = v_i - x_i \frac{\langle x_i v_i \rangle}{\langle x_i^2 \rangle}$$

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

$$k_B T_i(t) = m \frac{\varepsilon_i^2(t)}{\langle x_i^2 \rangle}.$$

**Equilibrium Temperature**

With $k_B T_{x,b} = m \langle \langle \Delta v_{x,b} \rangle^2 \rangle$, 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 $T_z$

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

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

$$T_x > T_{\text{eq}} \iff T_y < T_{\text{eq}}$$

and vice versa.

**Emittance Growth Rates**

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

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

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

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

The change of the emittance may be positive as well as negative.

**Entropy**

Summing over all three degrees of freedom, we get

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

$\therefore$ The change of the “total emittance” is always positive

$\therefore$ $S$ has the character of an entropy within a closed system

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

$$\tau_{\text{ef}}^{-1} = \frac{1}{3} \beta f (l_{xy} + l_{xz} + l_{yz}), \quad \varepsilon = \frac{\beta f}{3} \varepsilon_x \varepsilon_y \varepsilon_z$$

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

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

We will see that this description also applies to computer noise effects in simulations of charged particle beams.
With the abbreviations
\[
\begin{align*}
  a &= \sqrt{\langle x^2 \rangle} \\
  b &= \sqrt{\langle y^2 \rangle} \\
  \delta &= \sqrt{\langle (\Delta p/p)^2 \rangle} \\
  D &= \Delta x / (\Delta p / p) \\
  \eta &= \gamma^{-2} - D / \rho \\
  A &= \sqrt{a^2 + D^2 \delta^2} \\
  K &= 2 Ze_0 I / (4\pi \epsilon_0 mc^3 \beta \gamma^3)
\end{align*}
\]

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:

\[
\begin{align*}
  \ddot{a} + \beta_f \dot{a} + \omega_x^2 a - \frac{K/2}{A(A + b)} a - \frac{\varepsilon_x^2}{a^3} &= 0 \\
  \ddot{b} + \beta_f \dot{b} + \omega_y^2 b - \frac{K/2}{A + b} b - \frac{\varepsilon_y^2}{b^3} &= 0 \\
  \ddot{D} + \left( \omega_x^2 - \rho^{-2} \right) D - \frac{K/2}{A(A + b)} D - \frac{1}{\rho} &= 0 \\
  \frac{1}{a^2} \frac{d}{dt} a^2 + \frac{2}{3} \beta_f \left( 2 \frac{\varepsilon_x^2}{a^2} - \frac{\varepsilon_y^2}{b^2} - \eta \delta^2 \right) &= 0 \\
  \frac{1}{b^2} \frac{d}{dt} b^2 + \frac{2}{3} \beta_f \left( 2 \frac{\varepsilon_y^2}{b^2} - \frac{\varepsilon_x^2}{a^2} - \eta \delta^2 \right) &= 0 \\
  \eta \frac{d}{dt} \delta^2 + \frac{2}{3} \beta_f \left( 2 \eta \delta^2 - \frac{\varepsilon_x^2}{a^2} - \frac{\varepsilon_y^2}{b^2} \right) &= 0
\end{align*}
\]
Irreversibility in Computer Simulations

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

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

Transformation that reverses the direction of time flow:

$$ t \rightarrow -t \quad \Rightarrow x_i \rightarrow x_i, \quad v_i \rightarrow -v_i. $$

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

$$ L_{FP} = L_{rev} + L_{ir}. $$

The reversible operator $L_{rev}$: terms that change sign under time reversal, hence leave $\frac{\partial f}{\partial t} = L_{rev} f$ invariant.

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

$$ L_{rev} = \sum_{i=1}^{3} \left[ -\frac{\partial}{\partial x_i} v_i - \frac{1}{m} \frac{\partial}{\partial v_i} \left( F_{ext,i} + qE_{sc,i}^{sm} \right) \right]. $$

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

The components that do not change sign make up $L_{ir}$

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

$L_{ir}$ 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.
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.

Emittance growth factors versus number of cells obtained by 2-dimensional particle-in-cell simulations of beam transport channels. No overall growth occurs for zero temperature difference ($T_x = T_y$).

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.
- 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 ($\beta_f = 0$).