Analytical approaches for the dynamics of charged particle beams

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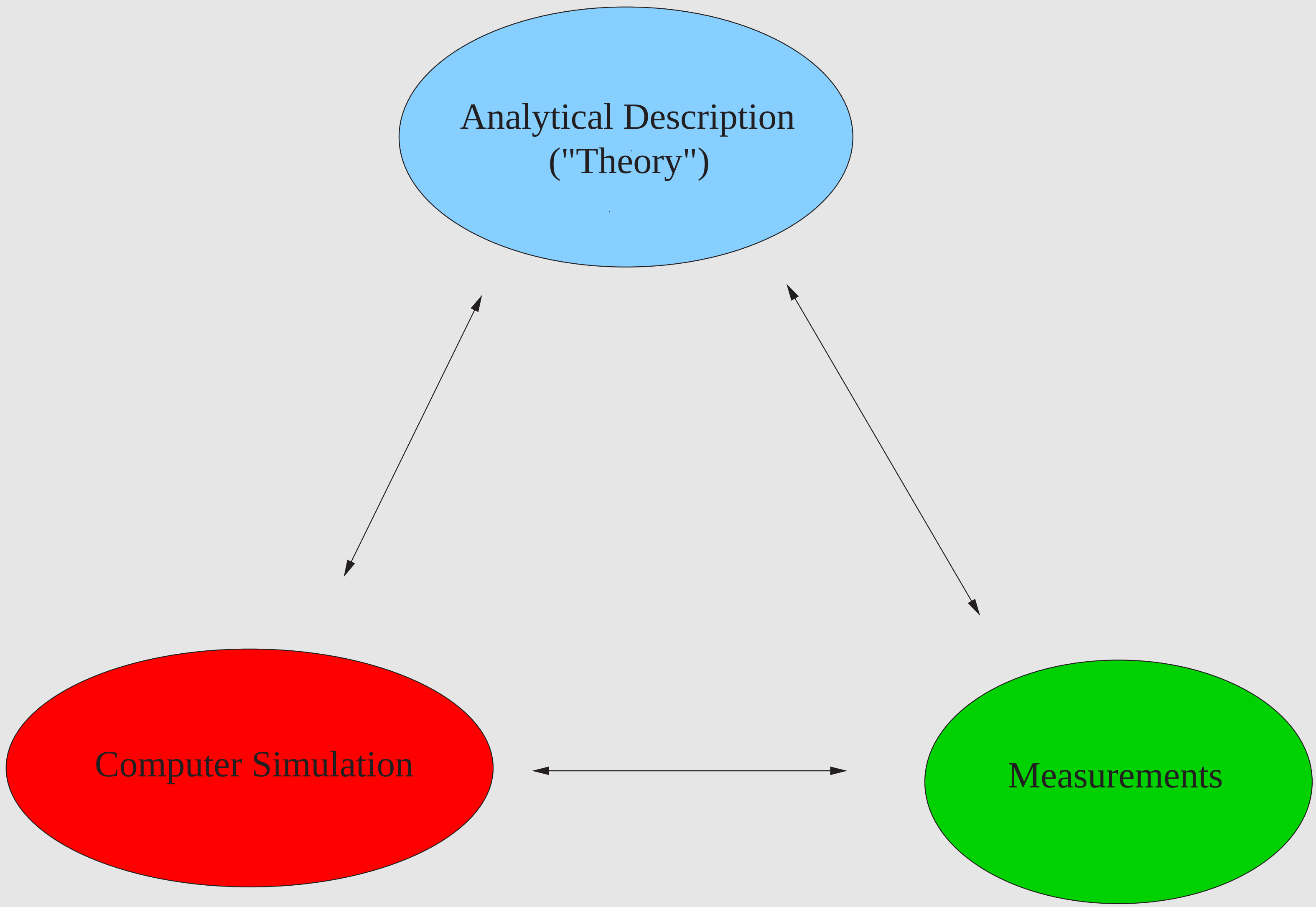
Outline

- Review: Hamiltonian mechanics of N particle systems
- Liouville's theorem
- Continuous description of beam dynamics
- Vlasov equation
- Moment analysis of the Vlasov equation
- Beam envelope equations
- Comparison of "analytic", simulated, and measured quantities
- Remarks on irreversibility in computer simulations
- Outlook: "non-Liouvillean" effects

The "Three Pillars" of today's Physics



Hamilton mechanics: basis of our description of dynamical systems.

Hamiltonian H for a system of N (interacting) particles

$$H = \frac{m}{2} \sum_{i=1}^{N} \boldsymbol{v}_i^2 + V(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N, t)\,, \quad i = 1, \ldots , N$$

With H given, we obtain from Hamilton's variational principle the "canonical equations" for each $i = 1, \ldots , N$

$$\dot{\boldsymbol{x}}_i = \frac{\partial H}{\partial \boldsymbol{v}_i} = \boldsymbol{v}_i\,, \quad m\dot{\boldsymbol{v}}_i = -\frac{\partial H}{\partial \boldsymbol{x}_i} = -\frac{\partial V(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N, t)}{\boldsymbol{x}_i}$$

Together with the initial condition

$$\big(\boldsymbol{x}_1(t_0), \boldsymbol{v}_1(t_0), \ldots , \boldsymbol{x}_N(t_0), \boldsymbol{v}_N(t_0)\big)\,,$$

the system of N particles is *completely* determined by the — generally coupled — system of $6N$ first order differential equations.

Properties of this description

- deterministic: The system is fully determined, no sources exist that could cause loss of information on the system's state
- reversible: the equations of motion ("canonical equations") are invariant with respect to time-inversion transformations

$$t \to -t \qquad \leadsto \boldsymbol{x}_i \to \boldsymbol{x}_i, \qquad \boldsymbol{v}_i \to -\boldsymbol{v}_i\,.$$

  If we know the initial condition (at t_0) and the Hamiltonian, we can integrate the canonical equations to any instant of time, either $t > t_0$, or $t < t_0$
- The canonical equations form the basis for computer simulations. In most cases, we have $N_{\text{sim}} \ll N$ (representative sample).
- "Analytically hopeless": even the "three-body-problem" lacks an analytical solution.
- For analytical studies, simplifying assumptions are necessary.

Liouville's theorem

Liouville's theorem (proper) states that the volume element $d\Gamma$

$$d\Gamma = d\boldsymbol{x}_1 d\boldsymbol{v}_1 \ldots d\boldsymbol{x}_N d\boldsymbol{v}_N = d\boldsymbol{x}'_1 d\boldsymbol{v}'_1 \ldots d\boldsymbol{x}'_N d\boldsymbol{v}'_N$$

of a Hamiltonian N particle system is

invariant with respect to *canonical transformations*

— in particular with respect to the system's time evolution.
$\rightsquigarrow$ just a one invariant out of the set of Poincaré invariants.

We may easily proof Liouville's theorem by showing that the determinant of the Jacobi matrix associated with a canonical transformation is unity.

Note: the projection of $d\Gamma$ to subspaces — especially to the 6-dimensional phase space or 2-dimensional phase-space planes — does *not* necessarily provide a conserved quantity!

We must be very careful if we draw conclusions that apply to subspaces!

We summarize:

- The single particle approach with $N_{\text{sim}} \ll N$ is appropriate for computer simulations.
- It does not “work” for analytical studies.
- Alternative: description in terms of statistical mechanics
$\rightsquigarrow$ continuous description of beam dynamics.

Continuous description of beam dynamics

For the continuous description of the ion beam, we define a 6-dimensional phase-space probability density function

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

$\leadsto$ $f \, d\boldsymbol{x} \, d\boldsymbol{v}$ provides the probability of finding a particle inside the volume $d\boldsymbol{x} \, d\boldsymbol{v}$ around the phase-space point $(\boldsymbol{x}, \boldsymbol{v})$ at time t.

$\leadsto$ f is a smooth function of the phase-space variables.

$\leadsto$ f does *not* provide information on individual particles.

The “special” Liouville theorem

$$\frac{df}{dt} = 0$$

applies for systems with non-negligible Coulomb interaction only if

- the system can be described to sufficient accuracy by a *continuous* Hamilton function. This means that we must be allowed to treat the internal space charge forces analogously to an external force field.

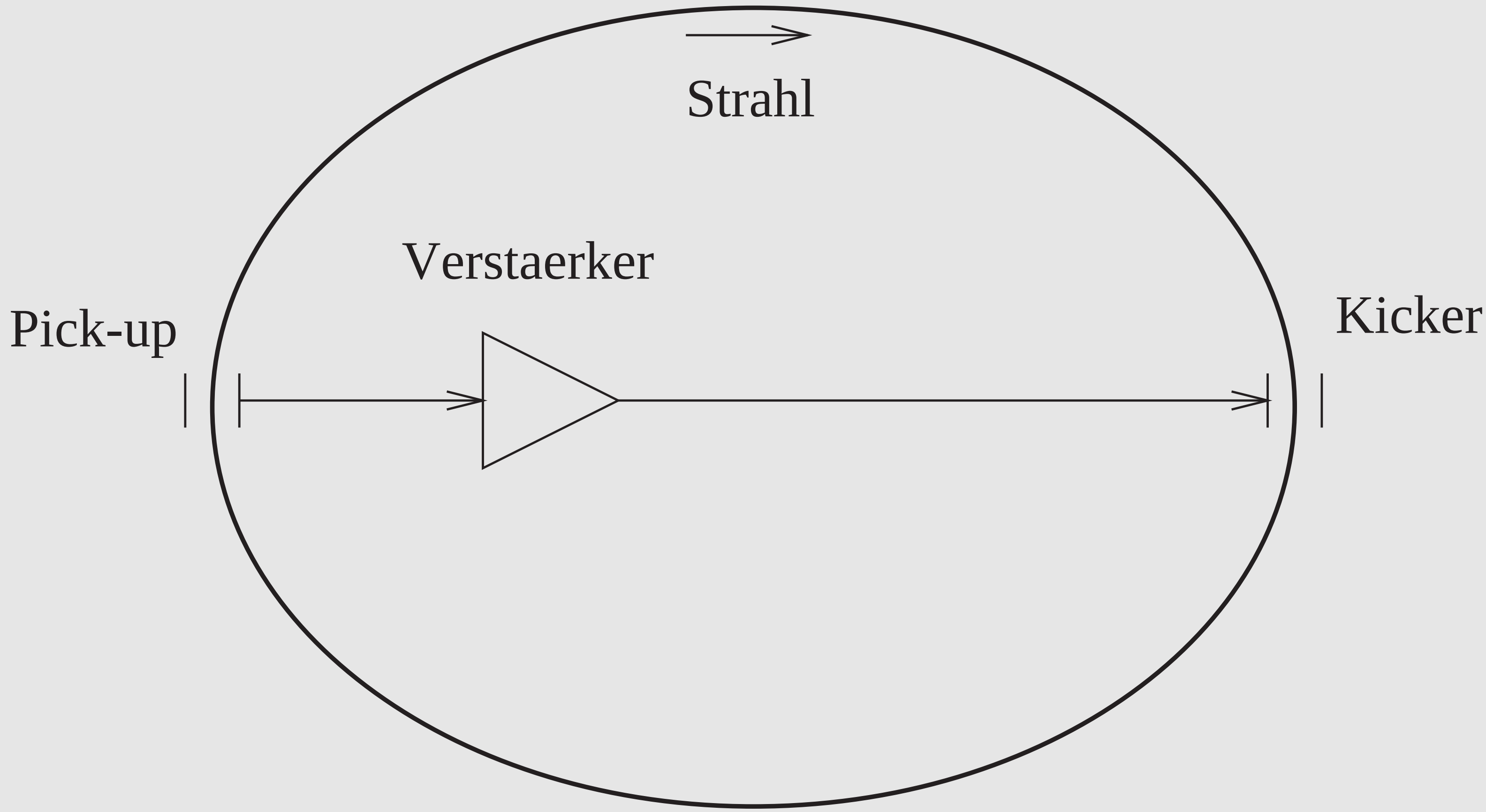
We observe:

The statistical description smoothes out the effects reflecting the actual charge granularity.

$\leadsto$ The usual equation of motion of the phase-space probability density $df/dt = 0$ does *not* cover intra-beam scattering effects, for example.

$\leadsto$ $df/dt = 0$ does not hold for “stochastic cooling”!

Remark on stochastic cooling



The cooling process hinges on charge density fluctuations within the beam that are sampled by a pick-up electrode. This signal is used to counteract the related momentum fluctuations within the beam at some specific point further downstream the ring.

$\leadsto$ The continuous description does not apply!

$\leadsto$ The “special” Liouville theorem for f does not hold, hence stochastic cooling does not conflict with Liouville’s theorem (in its special form).

Vlasov equation

Explicitly, the Liouville equation for $f(\boldsymbol{x}, \boldsymbol{v}, t)$ writes

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i} + \sum_{i=1}^{3} \ddot{x}_i \frac{\partial f}{\partial v_i} = 0\,,$$

Inserting $\ddot{\boldsymbol{x}}$, this equation is usually referred to as the “Vlasov” equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_x f + \tfrac{1}{m} \left(\boldsymbol{F}_{\mathrm{ext}} + q \boldsymbol{E}_{\mathrm{ssc}} \right) \cdot \nabla_v f = 0\,.$$

Herein $\boldsymbol{F}_{\mathrm{ext}}$ stands for the external forces applied to the beam by focusing elements (such as quadrupoles) and $\boldsymbol{E}_{\mathrm{ssc}}$ for the smooth part of the space-charge forces. $\boldsymbol{E}_{\mathrm{ssc}}$ depends on f via Poisson’s equation:

$$\operatorname{div} \boldsymbol{E}_{\mathrm{ssc}}(\boldsymbol{x}, t) = \frac{q}{\epsilon_0} \int f(\boldsymbol{x}, \boldsymbol{v}, t)\, d\boldsymbol{v}\,.$$

We summarize:

- The statistical description replaces the original problem of solving $6N$ coupled first-order equations by *one* equation of motion for the 6-dimensional probability density $f(\boldsymbol{x}, \boldsymbol{v}, t)$.
- The coupled set of Vlasov and Poisson equations provides the *closed equation of motion* for f if all effects due to the actual charge granularity can be neglected.
- Even this equation is generally not worth-while to solve directly.
- We do not really want to know $f(\boldsymbol{x}, \boldsymbol{v}, t)$ in detail.
- We must switch to even more global quantities in our analytical description of ion beams.

Moment analysis of the Vlasov equation

The usual way to switch to even more global physical quantities is to consider "moments" of $f(\boldsymbol{x}, \boldsymbol{v}, t)$

$$\langle x_i^2 \rangle (t) = \int x_i^2 \, f(\boldsymbol{x}, \boldsymbol{v}, t) \, d\boldsymbol{x} d\boldsymbol{v} \,, \quad i = 1, 2, 3 \,.$$

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

Idea: Instead of solving the equation of motion for f, we are going to set up and solve the equations of motion for the second beam moments.

The derivatives of the moments are calculated according to

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

inserting $\partial f / \partial t$ from the Vlasov-Poisson equation.

Integrating by parts, we obtain for each phase-space plane $i = 1, 2, 3$ a coupled set of "moment" equations

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

$$m\frac{d}{dt}\left\langle x_i v_i\right\rangle - m\left\langle v_i^2\right\rangle - \left\langle x_i F_{\mathrm{ext},i}\right\rangle - q\left\langle x_i E_{\mathrm{ssc},i}\right\rangle = 0$$

$$m\frac{d}{dt}\left\langle v_i^2\right\rangle - 2\left\langle v_i F_{\mathrm{ext},i}\right\rangle - 2q\left\langle v_i E_{\mathrm{ssc},i}\right\rangle = 0$$

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

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

The time derivative of the rms emittance may be arranged as

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

RMS beam envelope equations

For unbunched beams with elliptic cross section in real space, we have

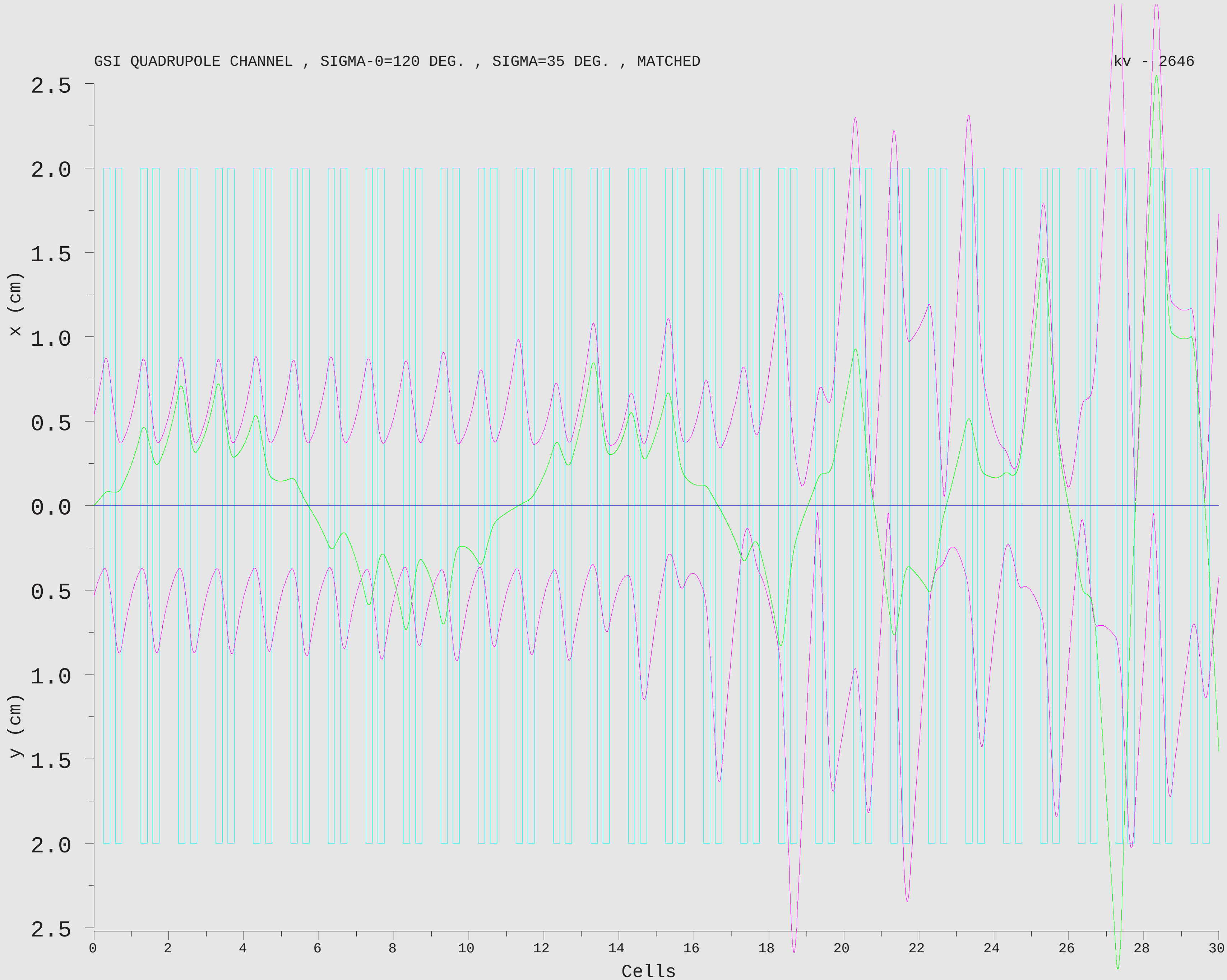
$$\langle x_i E_{\mathrm{sc},i} \rangle = \frac{I}{4\pi\epsilon_0 c\beta} \frac{\sqrt{\langle x_i^2 \rangle}}{\sqrt{\langle x^2 \rangle} + \sqrt{\langle y^2 \rangle}} \,.$$

We obtain the rms envelope equation from the first two moment equations

$$\frac{d^2}{dt^2}\sqrt{\langle x^2 \rangle} + \omega_x^2(t)\sqrt{\langle x^2 \rangle} - \frac{qI}{4\pi\epsilon_0 mc\beta} \frac{1}{\sqrt{\langle x^2 \rangle} + \sqrt{\langle y^2 \rangle}} - \frac{\varepsilon_x^2(t)}{\sqrt{\langle x^2 \rangle^3}} = 0$$

$$\frac{d^2}{dt^2}\sqrt{\langle y^2 \rangle} + \omega_y^2(t)\sqrt{\langle y^2 \rangle} - \frac{qI}{4\pi\epsilon_0 mc\beta} \frac{1}{\sqrt{\langle x^2 \rangle} + \sqrt{\langle y^2 \rangle}} - \frac{\varepsilon_y^2(t)}{\sqrt{\langle y^2 \rangle^3}} = 0 \,.$$

We must assume the rms emittances to be approximately *constant* to be able to integrate this coupled set.
$\leadsto$ valid for linear external forces and if no transient effects occur.


GSI QUADRUPOLE CHANNEL , SIGMA-0=120 DEG. , SIGMA=35 DEG. , MATCHED
kv - 2646
x (cm)
y (cm)
2.5
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
Cells

Comparison of "analytic", simulation, and measured quantities

In our analytic description, the "second moment" in x was defined as

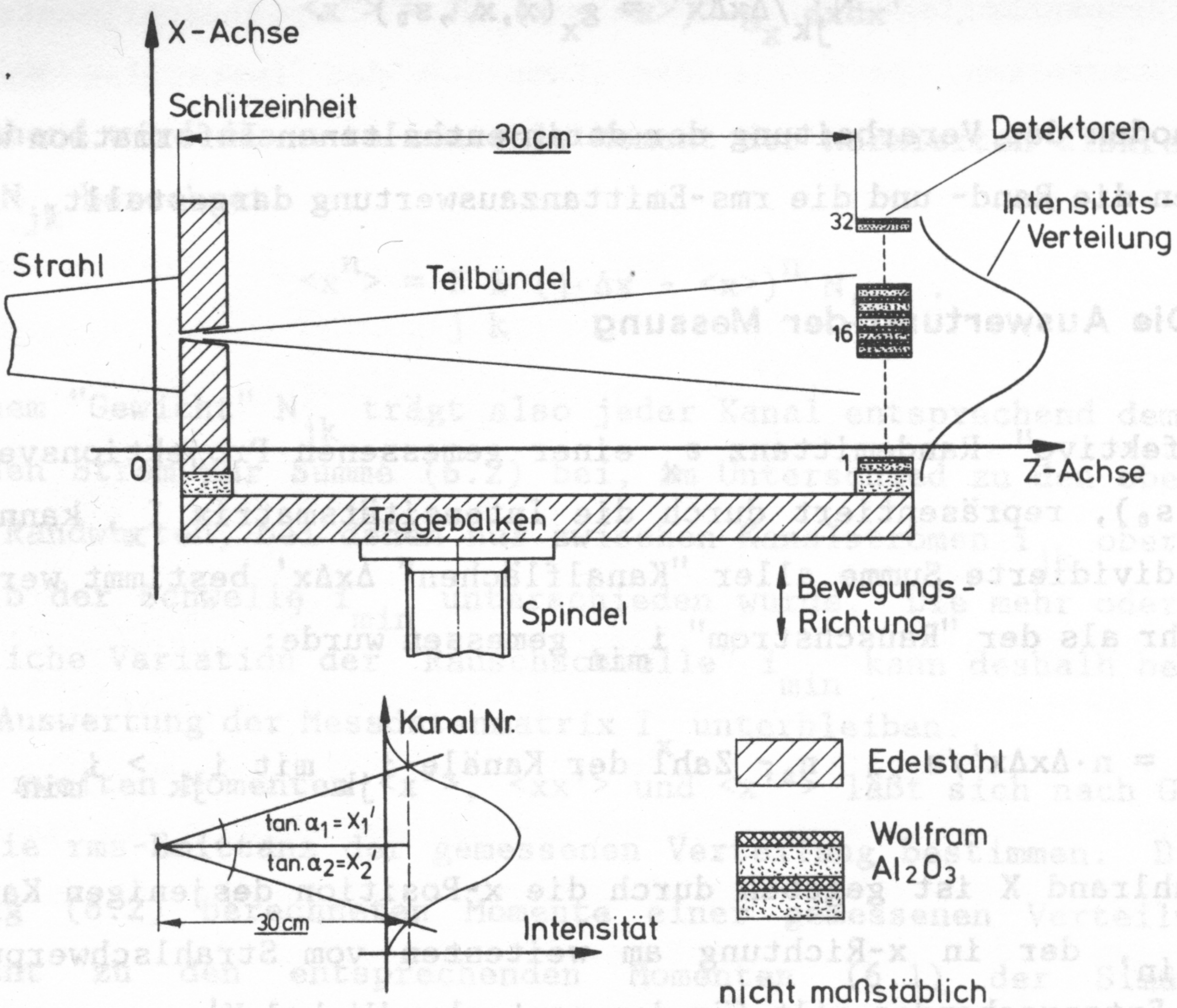
$$\langle x^2 \rangle = \int x^2 \, f(\boldsymbol{x}, \boldsymbol{v}, t) \, d\boldsymbol{x} d\boldsymbol{v} \, .$$

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

In a computer simulation based on N_{sim} representative particles, this quantity is given by

$$\langle x^2 \rangle = \frac{1}{N_{\text{sim}}} \sum_{i=1}^{N_{\text{sim}}} x_i^2 \, .$$

How do we measure this quantity?


X-Achse
Schlitzeinheit
30 cm
Detektoren
32
Intensitäts-
Verteilung
Strahl
Teilbündel
16
0
1
Z-Achse
Tragebalken
Bewegungs-
Richtung
Spindel
Kanal Nr.
tan. α1 = X1'
tan. α2 = X2'
30 cm
Intensität
Edelstahl
Wolfram
Al2O3
nicht maßstäblich

The result of such a “slit and detector” measurement is given by the “current matrix” $\boldsymbol{I}$

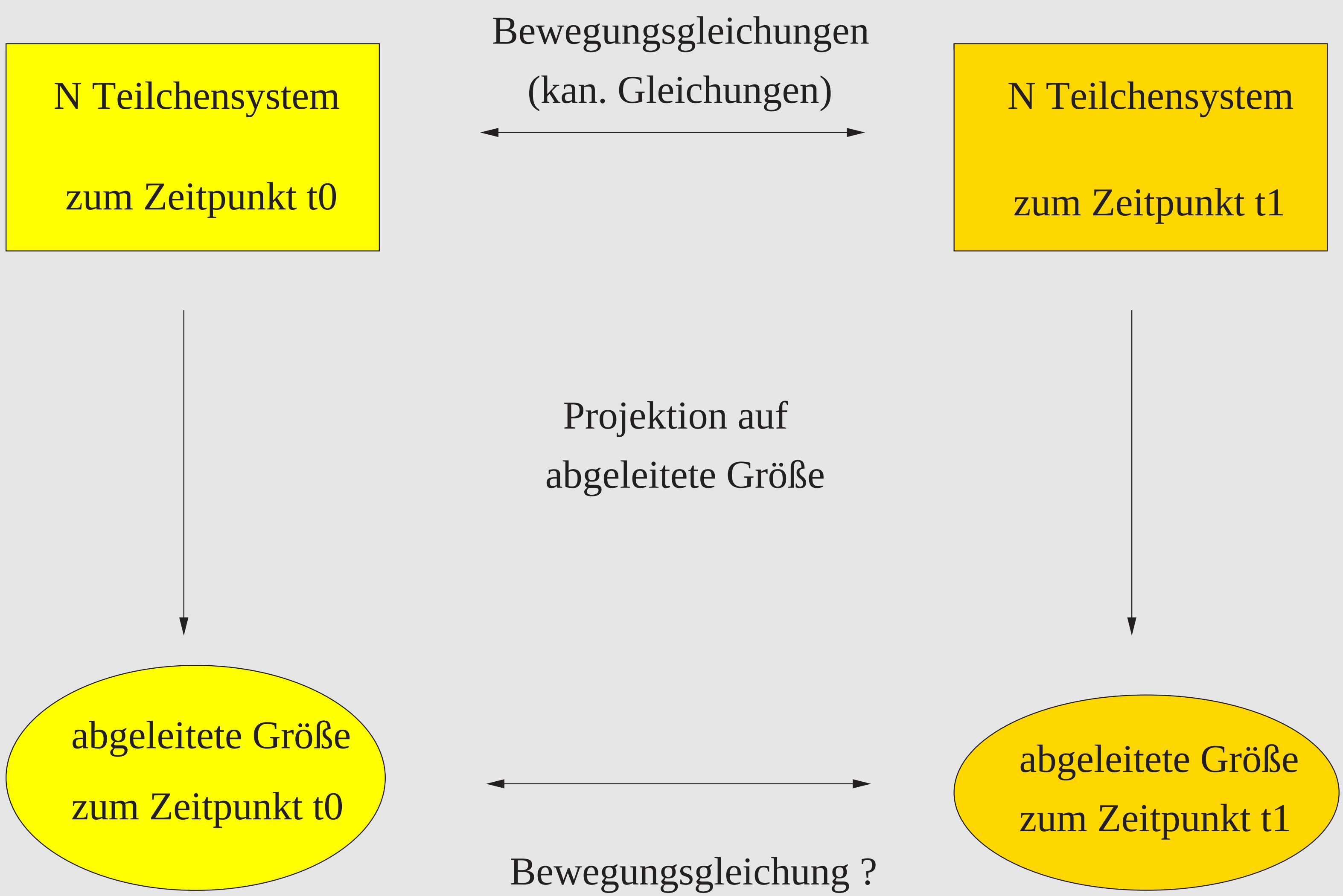
$$\boldsymbol{I} = \begin{pmatrix} i_{11} & \cdots & i_{1m} \\ \vdots & \ddots & \vdots \\ i_{n1} & \cdots & i_{nm} \end{pmatrix},$$

with m the number of slit positions, and n the number of detectors. For a fixed step size Δx of the slit positions, the second beam moments can now be directly calculated

$$\langle x^2 \rangle = I_{\mathrm{t}}^{-1} \sum_{j=1}^{m} \sum_{k=1}^{n} i_{kj} \Big(j\Delta x - \langle x \rangle \Big)^2 ,$$

with

$$I_{\mathrm{t}} = \sum_{j=1}^{m} \sum_{k=1}^{n} i_{kj} , \qquad \langle x \rangle = \sum_{j=1}^{m} \sum_{k=1}^{n} i_{kj} \, j \, \Delta x .$$


N Teilchensystem
zum Zeitpunkt t0
Bewegungsgleichungen
(kan. Gleichungen)
N Teilchensystem
zum Zeitpunkt t1
Projektion auf
abgeleitete Größe
abgeleitete Größe
zum Zeitpunkt t0
abgeleitete Größe
zum Zeitpunkt t1
Bewegungsgleichung ?

We summarize:

- We must clearly distinguish quantities that have only meaning at a fixed instant of time (“figures of merit”, like “90 % emittances”) from quantities that are related to the system’s equations of motion.
- If we want to understand the dynamics of measured quantities, we must ensure that these quantities are “physical” in the sense that they must be consistent with the equations of motion.
  $\leadsto$ an “equation of motion” must exist for the measured quantities!
- The rms description provides a basis to compare measured emittances, beam profiles, etc. with results of computer simulations and analytical approximations.
- The rms description avoids all problems that are associated with the definitions of boundaries.
  $\leadsto$ Best possible accuracy!

Remarks on irreversibility

Consider the transformation that reverses the direction of time flow:

$$t \longrightarrow -t \qquad \rightsquigarrow x_i \longrightarrow x_i, \qquad v_i \longrightarrow -v_i, \qquad \boldsymbol{E} \longrightarrow \boldsymbol{E}\,, \qquad \boldsymbol{B} \longrightarrow -\boldsymbol{B}.$$

We may investigate the single particle equations of motion with respect to this transformation

$$m\ddot{\boldsymbol{x}}_i - \boldsymbol{F}_{\text{ext}}(\boldsymbol{x}_i, t) - q\big(\boldsymbol{E}_i + \boldsymbol{v}_i \times \boldsymbol{B}_i\big) = 0\,, \qquad i = 1, \ldots, N_{\text{sim}}\,.$$

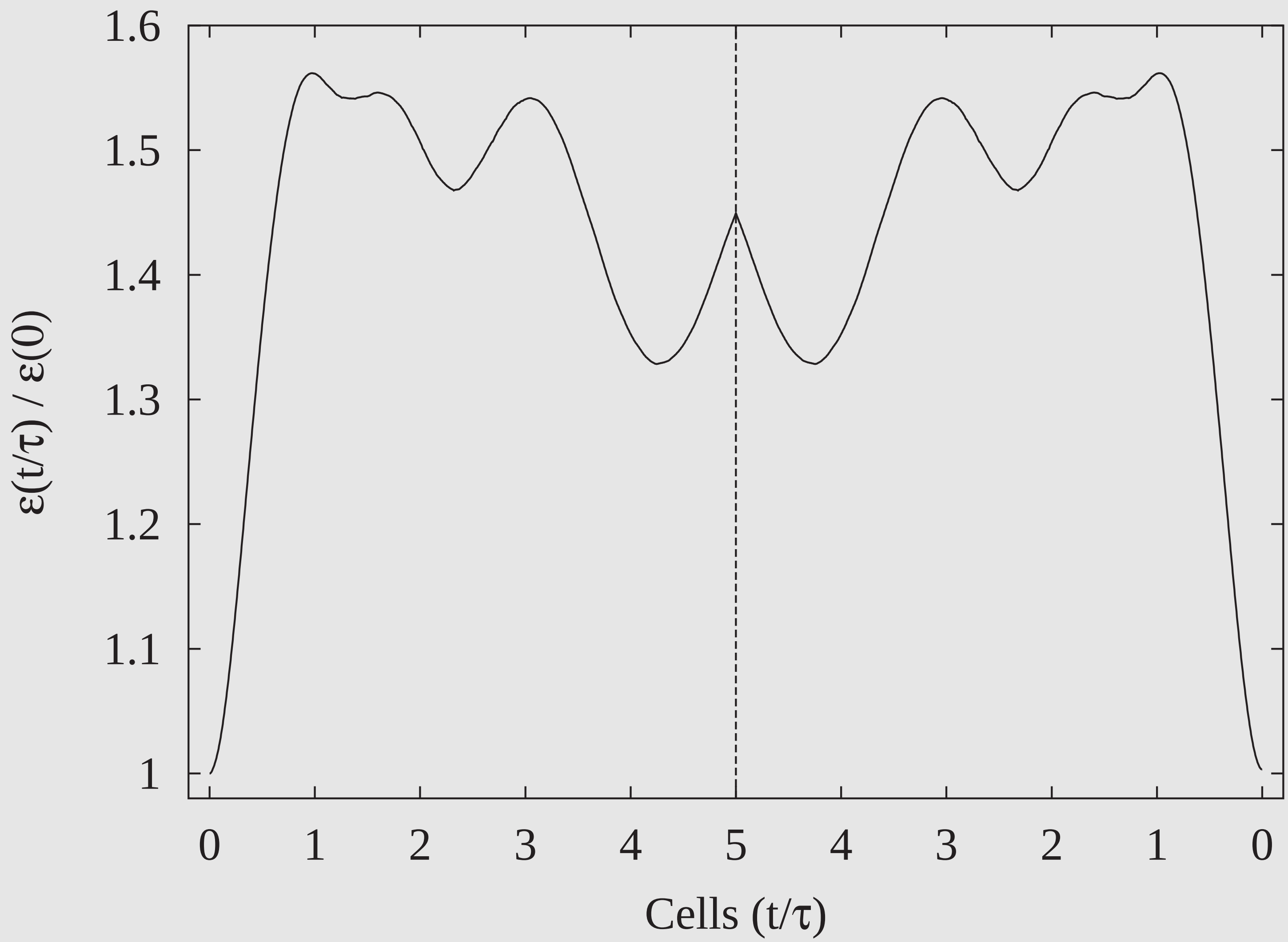
We observe that this equation is indeed invariant under time reversal.

$\rightsquigarrow$ We may convince ourselves that the Vlasov equation is also invariant.

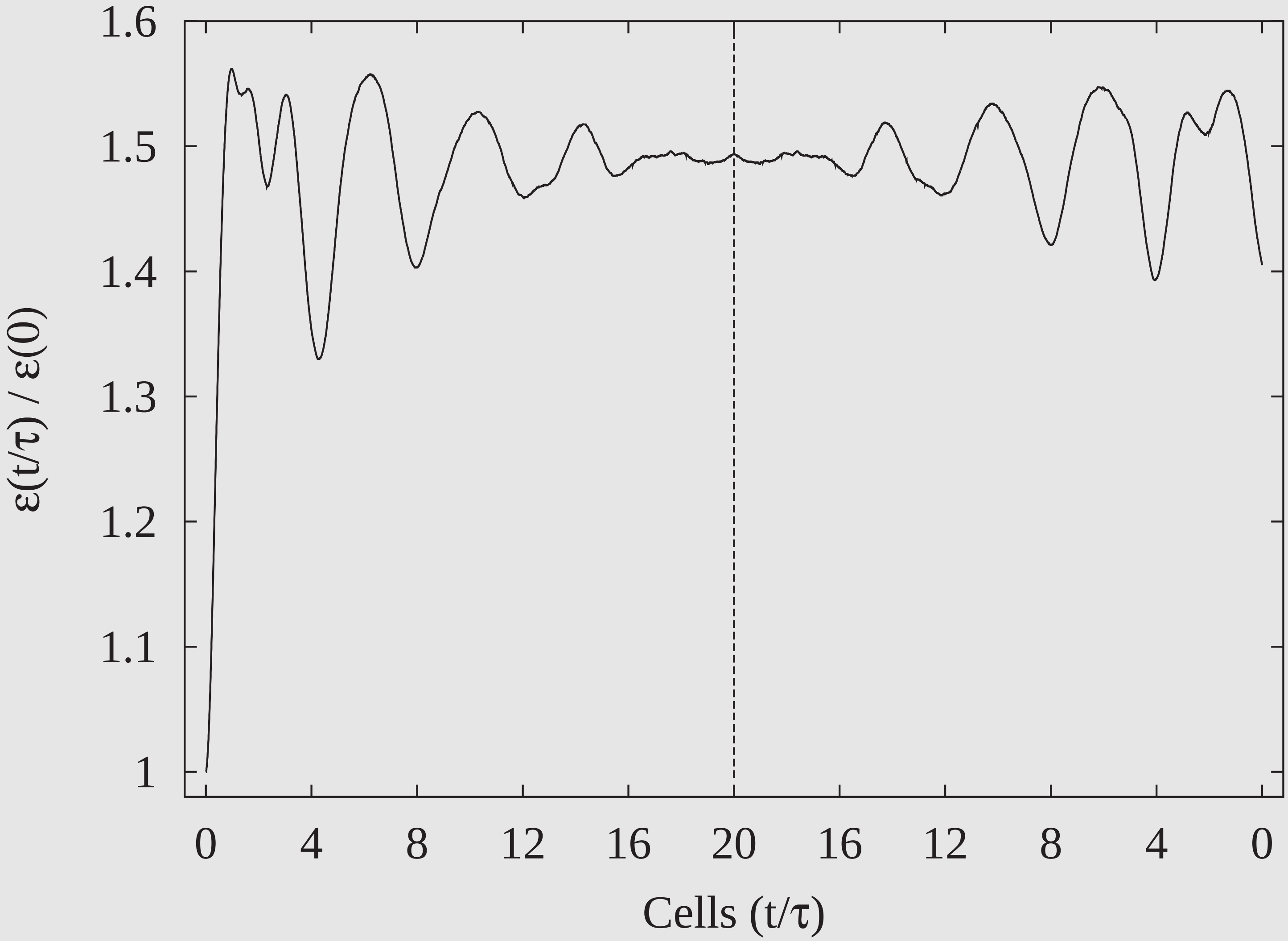
$\rightsquigarrow$ Earlier states are fully restored — just like a movie that is reversed.

$\rightsquigarrow$ The equations describe the *reversible* aspects of the system evolution.

But: computer simulations of dynamical systems are irreversible — even if the coded equations of motion are strictly reversible and the integration algorithm maintains the symplectic nature of the canonical equations (“symplectic integrator technique”).



1.6
1.5
1.4
1.3
1.2
1.1
1
ε(t/τ) / ε(0)
0 1 2 3 4 5 4 3 2 1 0
Cells (t/τ)


1.6
1.5
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ε(t/τ) / ε(0)
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4
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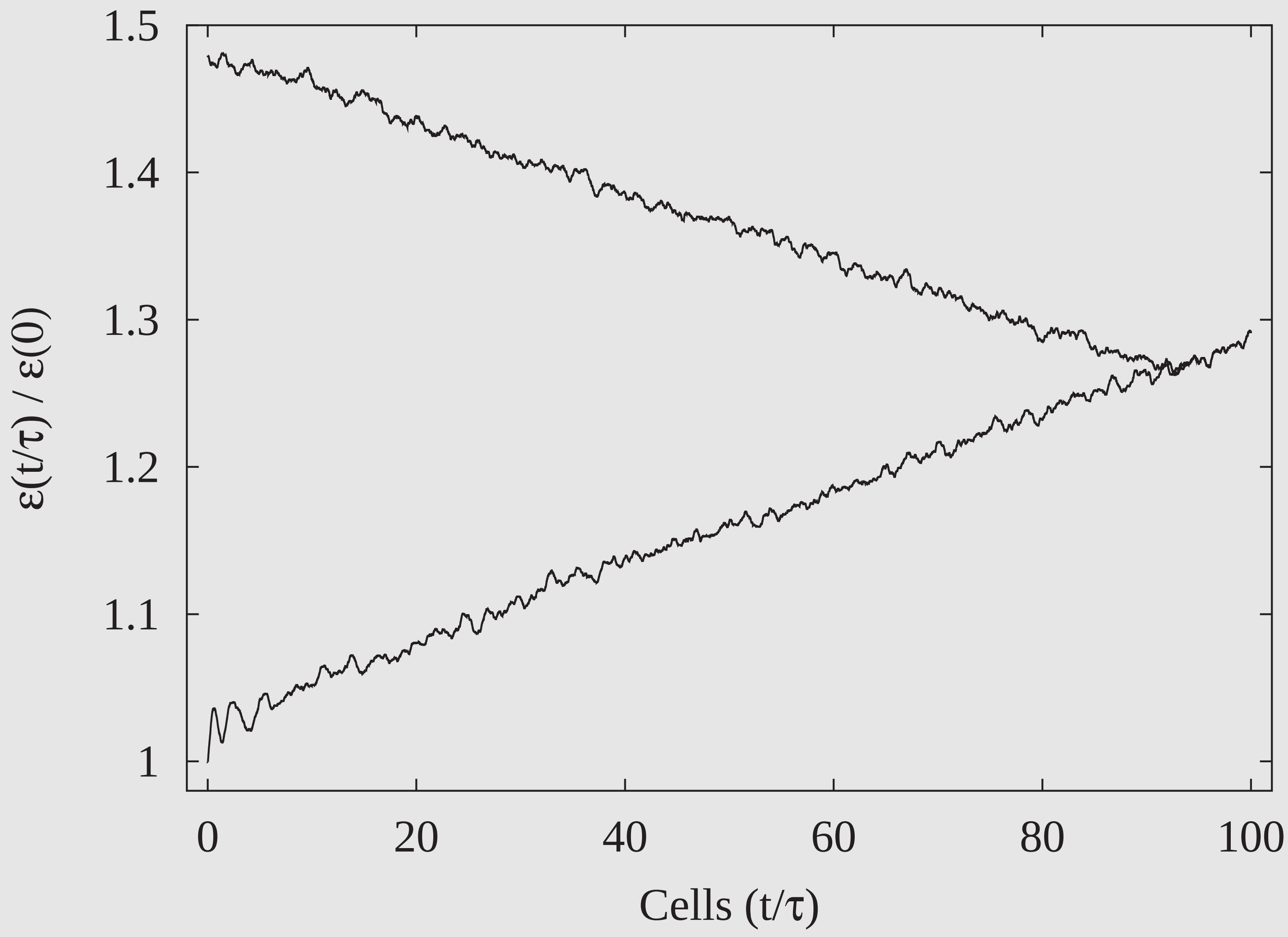
Cells (t/τ)



1.5
1.4
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1.2
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ε(t/τ) / ε(0)
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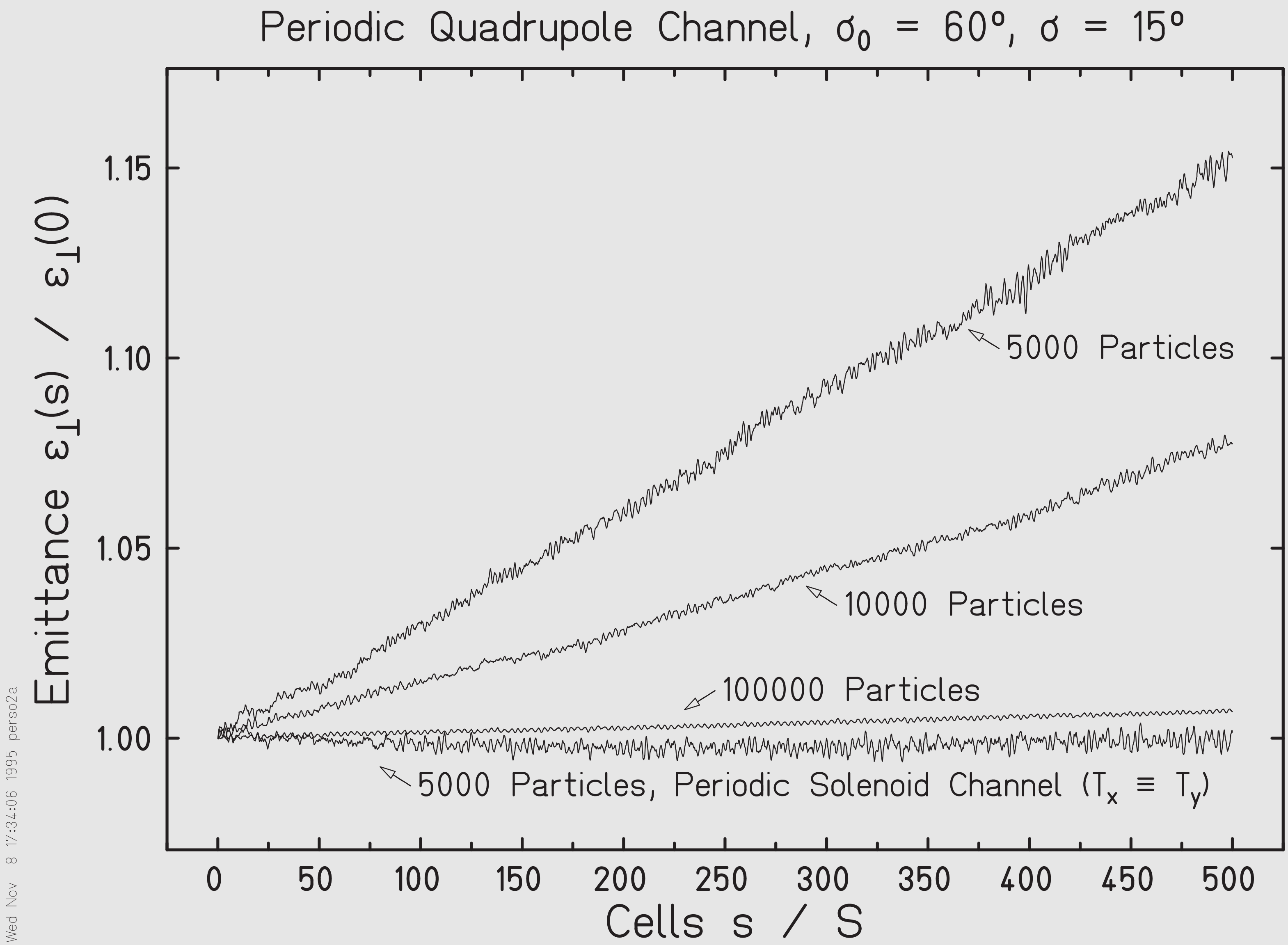
40
60
80
100
Cells (t/τ)


Periodic Quadrupole Channel, σ0 = 60°, σ = 15°
Emittance εT(s) / εT(0)
1.15
1.10
1.05
1.00
5000 Particles
10000 Particles
100000 Particles
5000 Particles, Periodic Solenoid Channel (Tx ≡ Ty)
0
50
100
150
200
250
300
350
400
450
500
Cells s / S
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“Non Liouvillean” Effects

$\rightsquigarrow$ An additional equation, hence a generalization of the “special” Liouville theorem is necessary (Chandrasekhar (1943)):

$$\frac{df}{dt} = 0 + \left[\frac{\partial f}{\partial t}\right]_{\mathrm{NL}} .$$

If the non-Liouvillean effects are small compared to the macroscopic forces (smooth space charge and external forces), we can describe them by the Fokker-Planck equation:

$$\left[\frac{\partial f}{\partial t}\right]_{\mathrm{NL}} = -\sum_i \frac{\partial}{\partial v_i}\left\{F_i(\boldsymbol{v},t)\, f\right\} + \sum_{i,j} \frac{\partial^2}{\partial v_i \partial v_j}\left\{D_{ij}(\boldsymbol{v},t)\, f\right\}$$

D_{ij} are referred to as elements of the “diffusion tensor” and the F_i as elements of the “drift vector” that describes the “dynamical friction forces”. They must be determined appropriately depending on the nature of the underlying physical process.

We summarize:

- The actual time evolution of the simulated system always comprises irreversible aspects — even if the actually coded equations of motion are strictly reversible.
- A computer simulation based on individual particles can never be an *exact* realization of a solution of the Vlasov equation.
- We must include these effects in our analytical description in order to fully understand our simulation results.