Hamiltonian Systems of Charged Particles in Discrete and Continuous Description

Habilitationsschrift

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„Denn wiewohl wir nur wenig von dieser Welt Vollkommenheit ausspähen oder erreichen werden, so gehört es doch zur Gesetzgebung unserer Vernunft, sie allwärts zu suchen und zu vermuten, und es muß uns jederzeit vorteilhaft sein, niemals aber kann es nachteilig werden, nach diesem Prinzip die Naturbetrachtung anzustellen“.

(Immanuel Kant, Kritik der reinen Vernunft)

Zusammenfassung

Die vorliegende Arbeit beschäftigt sich mit zeitabhängigen und nichtlinearen Hamiltonsystemen — sowohl in der exakten Beschreibung deterministischer Systeme mit n Freiheitsgraden, als auch in der kontinuierlichen Formulierung der statistischen Physik.

In Kapitel 1 betrachten wir Systeme wechselwirkender klassischer Teilchen mit n Freiheitsgraden. Wir blicken zunächst auf die Methode der kanonischen Transformation in der Beschreibung des „erweiterten Phasenraums“ zurück — in welchem die Zeit und die negative Hamiltonfunktion selbst als ein zusätzliches Paar kanonischer Variabler verwendet werden. Auf dieser Grundlage gelingt es dann, eine *Invariante* für eine allgemeine Klasse zeitabhängiger und nichtlinearer Hamiltonfunktionen abzuleiten.

Ein alternativer Ansatz diese Invariante zu erhalten, wird mit einem Rückblick auf das Noether-Theorem eingeleitet. Wir werden anschließend sehen, daß die Invariante genau einer Noether-Symmetrie entspricht.

Die Invariante selbst enthält die Gesamtheit aller kanonischen Variablen des Systems, sowie eine „Hilfsfunktion“ $\xi(t)$, welche ihrerseits einer homogenen, linearen Differentialgleichung dritter Ordnung genügen muß. Von speziellen isotropen, linearen Systemen abgesehen, hängen die Koeffizienten dieser Gleichung von den räumlichen Koordinaten aller Teilchen des Systems ab. Die Lösungsfunktion $\xi(t)$ läßt sich deshalb nur *gemeinsam* mit der Integration aller Bewegungsgleichungen ermitteln. Aufgrund dieser Tatsache führt die Existenz der Invarianten nicht zur Vereinfachung einer Berechnung der Systembewegung. Es zeigt sich, daß die Invariante als die konstante Anfangsenergie des Systems aufgefaßt werden kann, d.h. als die augenblickliche Systemenergie einschließlich aller im Verlauf seiner zeitlichen Entwicklung zu- und abgeführten Energienanteile.

Als Beispiele werden wir den gedämpften, zeitabhängigen harmonischen Oszillator, einen zeitabhängigen nichtlinearen Oszillator und ein dreidimensionales System von Coulomb-wechelwirkenden Teilchen in einem linearen, zeitabhängigen äußeren Potential betrachten. Für das letzte Beispiel wird gezeigt, daß die Invariante zur Abschätzung der Genauigkeit einer Computersimulation eines solchen Systems dienen kann. Als noch offene Frage wird der Fall eines instabilen Verhaltens der Hilfsfunktion $\xi(t)$ angesprochen. Es steht zu vermuten, daß hiermit ein Übergang von einer regulären zu einer chaotischen Entwicklung des Systems aufgezeigt wird.

Im zweiten Kapitel wechseln wir zu einer kontinuierlichen Behandlung von Hamiltonsystemen, welche aus einer riesigen Anzahl von Freiheitsgraden bestehen. Wie üblich bildet anstelle des Satzes gekoppelter Einzelteilchengleichungen die Bewegungsgleichung für die Wahrscheinlichkeitsdichte f des Phasenraums die Grundlage der Beschreibung. Die zeitliche Entwicklung des gegebenen Vielteilchensystems wird demnach durch die Lösung der Bewegungsgleichung für f — der Liouville-Gleichung — angenähert. Wir vereinfachen somit die Beschreibung des Systems, indem wir auf das Wissen über die Phasenraumposition einzelner Teilchen verzichten.

Für die meisten Fälle ist die in der Wahrscheinlichkeitsdichte f enthaltene Information über

das System ausreichend. Wir müssen jedoch im Auge behalten, daß die Liouville-Gleichung wegen ihrer Invarianz gegenüber Zeitumkehrtransformationen uns auf die reversiblen Aspekte der Dynamik beschränkt. Eine derartige Beschreibung genügt nicht mehr, wenn wesentliche Aspekte der zeitlichen Entwicklung des Systems durch den letztendlich individuellen Charakter der Teilchen bestimmt werden. Als Beispiel wird die Beschreibung elastischer Coulomb-Stöße in Ionenstrahlen („intra-beam scattering“) behandelt. Die Grundlage der Beschreibung dieses Effekts wird durch die kombinierte Vlasov-Fokker-Planck Gleichung gelegt. Unter Verwendung der Boltzmann-Entropie wird gezeigt, daß eine Entropiezunahme stets mit Wärmeaustausch innerhalb des Strahls verbunden ist.

Eine direkte Integration der Vlasov-Fokker-Planck Gleichung ist nicht erforderlich, wenn wir nur an globalen Systemvariablen, wie z.B. der zeitlichen Entwicklung von Emittanz und Impulsunschärfe, interessiert sind. Stattdessen genügt es, aus der Bewegungsgleichung für f Gleichungen für die „Momente von f“ abzuleiten. Wir werden sehen, daß auf diese Weise ein gekoppeltes System von Enveloppen- und Emittanzgleichungen entsteht, welches den Effekt der Emittanzvergrößerung durch Coulomb-Stöße in Speicherringen beschreibt. Es zeigt sich, daß die Wachstumsraten für Emittanz und Impulsunschärfe in dieser Beschreibung nur durch zwei Größen bestimmt werden: durch den Reibungskoeffizienten β_{fr}, welcher durch die globalen Strahlparameter bestimmt wird, und die gemittelte Temperaturanisotropie, als Funktion der gegebenen Ringoptik. Zur Überprüfung dieser Beschreibung werden die Ergebnisse der numerischen Integration des gekoppelten Satzes von Momentengleichungen mit Messungen der Gleichgewichtsemittanzen am Heidelberger Testspeicherring (TSR) verglichen.

Im dritten Kapitel werden wir uns der Ergebnisse der ersten beiden Kapitel bedienen, um das Auftreten irreversibler Effekte in Computer-Simulationen wechselwirkender Vielteilchensysteme zu analysieren und quantitativ zu beschreiben. Auch wenn nämlich die in unseren Simulationsprogrammen kodierten Bewegungsgleichungen reversibel sind, so sind ihre numerischen Integrationen *nicht* reversibel aufgrund der mit jeder Gleitkommaoperation verbundenen Ungenauigkeit. Das Entstehen von Irreversibilität in Computersimulationen Coulomb-wechselwirkender Teilchen wird demonstriert, indem wir eine Teilchenwolke unterschiedlich lange Strecken vorwärts und anschließend zum Startpunkt zurück transformieren.

Wir werden diese Ungenauigkeiten als „numerisches Rauschen“ interpretieren und dessen Wirkung auf die Teilchengesamtheit wieder durch die Fokker-Planck Gleichung beschreiben. Analog zu Kapitel 2 zeigt ihre Momentenanalyse, daß die zu erwartenden Wachstumsraten der Emittanz eines simulierten Systems Coulomb-wechselwirkender Teilchen durch zwei voneinander unabhängige Größen bestimmt wird. Zum einen ist dies die „Körnigkeit“ des Systems, welche maßgeblich durch die Anzahl der verwendeten Simulationsteilchen bestimmt wird. Zum anderen werden die theoretisch zu erwartenden makroskopischen Effekte durch das „Temperaturungleichgewicht“ innerhalb der Teilchenwolke bestimmt.

Die Ergebnisse unserer Simulationen folgen in der Tat diesen Voraussagen. Simulationen von Systemen mit verschwindender Temperaturanisotropie zeigen praktisch kein Wachstum der Emittanzen — auch wenn die Körnigkeit des Systems aufgrund geringer Zahl der Simulationsteilchen groß ist. Andererseits erhalten wir in Simulationen von Systemen mit endlicher Temperaturanisotropie deutliche Wachstumsraten der Emittanz — in starker Abhängigkeit von der Zahl der Simulationsteilchen, also der Körnigkeit des simulierten Systems. Das bisher ungeklärte Auftreten von Emittanzwachstumseffekten in der Simulation von Strahltransportkanälen kann somit als makroskopische Folge vieler kleiner Rundungsfehler, welche unsere Simulationen unvermeidlich begleiten, erklärt werden.

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Contents

Introduction

The present work deals with time-dependent and non-linear Hamiltonian systems of interacting particles in both the exact deterministic description and the continuous description in the framework of statistical mechanics. In most cases, the examples refer to systems of Coulomb-interacting particles. Yet, the results are of general validity and can also be applied to other classes of interaction forces.

The first chapter starts with a review of the technique of canonical transformations in the "extended phase space" — where the time and the negative Hamiltonian are taken as an additional pair of canonically conjugate coordinates. As will be shown, this formalism can be used to unveil invariants for time-dependent Hamiltonian systems. The reason behind the strategy is that we always learn about fundamental system properties from its invariants. For instance, in the case of an autonomous Hamiltonian system the Hamiltonian itself represent an invariant — which can be identified with the energy conservation law.

This direct way to acquire an invariant no longer exists in the general case of explicitly time-dependent systems, as invariants that depend on the canonical coordinates only do not exist for this class of Hamiltonian systems. We shall present a generalized method to determine invariants of n-degree-of-freedom Hamiltonian systems with non-linear and explicitly time-dependent potentials in Section 1.2.1, and in an even more general form in Section 1.6.1.

Another approach to work out the symmetries and the associated invariants of dynamical systems has been formulated in the pioneering work of S. Lie [1]. Based on his work, E. Noether [2] found the more specific invariants for differential equations that follow from variational problems. In Section 1.2.2, we shall review her famous theorem for dynamical systems whose equations of motion can be derived from Hamilton's variational principle. Furthermore, its representation in the framework of Hamilton's formulation of mechanics will be presented. For the particular class of time-dependent Hamilton-Lagrange systems covered in Section 1.2.1, the invariant derived from Noether's theorem is shown to agree with the invariant of the canonical transformation technique.

The invariant comprises both the canonical coordinates and an auxiliary function, which follows from a homogeneous, linear third-order auxiliary equation. Apart from isotropic linear systems, the coefficients of the auxiliary equation depend on all spatial particle coordinates. As the consequence, this differential equation can only be integrated in conjunction with the system's equations of motion. This enhanced complexity of the general auxiliary equation reflects — little surprisingly — the involved nature of a conserved quantity for time-dependent non-linear Hamiltonian systems. From the energy balance equation for time-dependent Hamiltonian systems, it is shown that the invariant can be interpreted as the sum of the system's time-varying energy content and the energy fed into or detracted from it.

As illustrative examples, we derive the invariant for three specific systems in Section 1.4, namely for the time-dependent damped harmonic oscillator, the time-dependent anharmonic undamped oscillator, and a three-dimensional system of Coulomb-interacting particles that is confined within a time-dependent quadratic external potential. For the last example, the invariant is applied to estimate the accuracy of a computer simulation of this system.

In the second chapter, we switch from the exact description of interacting particles to a statistical description that is appropriate for systems with a very large number of degrees of freedom. We hereby replace the system's description in terms of a huge number of coupled single particle equations of motion by the equation of motion of a probability density. By virtue of this description, the information on the particle ensemble is reduced to the knowledge of this probability density, which means that all information on individual particles is dropped.

For the greatest part of problems of practical interest, the equation of motion for the probability density is given by the Vlasov equation [3]. Because of the invariance of Vlasov's equation with respect to time reversal [4], we must be aware that it restricts our analytical framework to only reversible aspects of beam dynamics. However, a reversible, continuous description of beam dynamics no longer applies if the individual interactions of the point charges must be taken into account. Effects of elastic Coulomb scattering like the well-known phenomenon of intra-beam scattering [5] — observed for intense beams that circulate in storage rings — falls into this category. In order to include these irreversible effects into our analytical description of beams, the Vlasov approach must be generalized appropriately [6]. This will be achieved by separating the actual forces that act on the beam particles into a smooth macroscopic and a microscopic, fluctuating component. We will review this transition in detail in Section 2.2.1.

In Section 2.3, we will introduce the concept of Boltzmann entropy, given as a function of the phase-space density function. This quantity will then serve as a means to identify beam dynamics phenomena that are inherently irreversible and are hence associated with an increase of entropy. It will be shown that this entropy remains conserved as long as the evolution of the probability density complies with Liouville's equation. Entropy changes thus directly reflect the occurrence of non-Liouvillean effects — which in turn will be described by the Fokker-Planck equation. On this basis, we will show that entropy growth is directly related to heat transfers between different degrees of freedom within the beam.

If we are interested in the evolution of global beam characteristics — such as emittance and momentum spread — a direct integration of the Fokker-Planck equation is usually not worthwhile. One approach to simplify the analytical description of beam optics has been presented by Lapostolle [7] and Sacherer [8], deriving equations of motion for the "root-mean-square" beam moments from the Vlasov equation. In Section 2.4.1, we extend this technique deriving a generalized set of moment equations from the Fokker-Planck equation. We thus obtain additional terms in the equations for the beam moments that allow us to describe irreversible effects within the beam not covered by the Vlasov approach. With the Fokker-Planck coefficients for particles interacting weakly through an inverse square force law [9], we will use this moment description to estimate intra-beam scattering effects for the particular lattice of the Heidelberg heavy ion storage ring TSR. The obtained numerical results will be compared to measurements in order to verify the accuracy of our approach.

Owing to the fact that an analytical solution for the problem of particles interacting by Coulomb forces does not exists, computer simulations have become the tool of choice for the study of charged particle beams. In these studies, the actual beam is represented by an ensemble of simulation particles. A simulation thus means to numerically integrate the coupled set of equations of motion constituted by the particle ensemble and the beam optical lattice. Although the equations of motion of individual particles are invariant with respect to time reversal, the evolution of the particle ensemble is inevitably rendered irreversible because of the limited accuracy of numerical methods. Therefore, a simulation based on individual particles can never be a strict realization of a solution of the associated Vlasov equation.

With the knowledge of Chapters 1 and 2, we are given the means to describe the emerging of irreversibility and its consequences in computer simulations of systems of interacting particles. The idea pursued in Chapter 3 is to describe these "computer noise" effects analogously to random force effects emerging within the granular charge distribution of a "real" beam. We can then interpret the simulation results within the framework of the Fokker-Planck approach of Chapter 2.

This allows us to separate effects caused by the specific realization of the computer simulation from the “real beam” physics. The onset of irreversibility in a computer simulation of a charged particle ensemble will be demonstrated in Section 3.2.1 by a numerical transformation forward in time that is followed by the backward transformation to its starting point. For a specific time span after a numerical time reversal, the beam evolution behaves reversible. After this, the irreversible “computer noise” effects prevail, indicated by a sharp change of the sign of the emittance growth rate.

In Sections 3.2.4 and 3.2.4, we will analyze the numerical emittance growth factors obtained for different focusing lattices and numbers of simulation particles. It will be shown that the specific emittance growth rates emerging in these simulations can indeed be explained within the framework of the Fokker-Planck approach. This will enable us to distinguish “computer noise” related effects from those occurring within a real beam.

Chapter 1

Hamiltonian systems of discrete particles

An invariant for general non-linear and time-dependent Hamiltonian systems of interacting particles will be derived in this chapter. We will discuss its physical meaning and also provide numerical examples. Furthermore, possible applications will be addressed.

1.1 Hamilton's mechanics in the extended phase space

1.1.1 Concept of the extended phase space

We consider an n-degree-of-freedom system of classical particles that may be described in a $2n$-dimensional Cartesian phase space by an — in general — explicitly time-dependent Hamiltonian $H = H(\vec{q}, \vec{p}, t)$. Herein, $\vec{q}$ denotes the n-dimensional vector of the configuration space variables, and $\vec{p}$ the vector of conjugate momenta. The system's time evolution, also referred to as the phase-space path $(\vec{q}(t), \vec{p}(t))$, can be visualized as a curve in the $2n$-dimensional phase space. If the system's state is known at two distinct instants of time t_1 and t_2, the system's actual phase-space path between these fixed times is known to obey Hamilton's variation principle

$$\delta \int_{t_1}^{t_2} \left[\sum_{i=1}^{n} p_i(t) \frac{dq_i(t)}{dt} - H(q_1, \ldots, q_n; p_1, \ldots, p_n, t) \right] dt = 0 \,. \tag{1.1}$$

This variation integral (1.1) can easily be shown to vanish exactly if the "canonical equations"

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \,, \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \,, \qquad i = 1, \ldots, n \tag{1.2}$$

are satisfied. We observe that the time t plays the distinguished role of an external parameter which is contained in both the system path and the Hamiltonian H itself. As will be worked out in the following, this distinguished role of the time t may not be desirable in the general case of explicitly time-dependent (non-autonomous) Hamiltonian systems. We therefore introduce an evolution parameter s that parameterizes the system's time evolution $t = t(s)$. With s the new integration variable, we may rewrite Hamilton's principle (1.1) as [10, 11]

$$\delta \int_{s_1}^{s_2} \left[\sum_{i=1}^{n} p_i(s) \frac{dq_i(s)}{ds} - H\big(\vec{q}(s), \vec{p}(s), t(s)\big) \frac{dt(s)}{ds} \right] ds = 0 \,. \tag{1.3}$$

With this symmetric form of the integrand, it looks reasonable to conceive the time in conjunction with the negative Hamiltonian as an additional pair of canonically conjugate coordinates. We thus introduce in a natural way the $(2n+2)$-dimensional "extended" phase space by defining

$$q_{n+1} = t\,, \qquad p_{n+1} = -\mathcal{H}$$

as additional phase-space dimensions. Provided that the Hamiltonian $H(\vec{q},\vec{p},t)$ represents the sum of the system's kinetic and potential energies, then $\mathcal{H}$ is understood as an s-dependent variable that measures the instantaneous energy content of the Hamiltonian system H

$$\mathcal{H}(s) = H\big(\vec{q}(s),\vec{p}(s),t(s)\big)\,. \tag{1.4}$$

A Hamiltonian $\widetilde{H}$ pertaining to the extended phase space that carries the information of H on the dynamics of the given system may be defined as an implicit function $\widetilde{H}$ of the extended phase-space variables

$$\widetilde{H}(\vec{q},\vec{p},t,\mathcal{H}) = \big(H(\vec{q},\vec{p},t) - \mathcal{H}\big)\frac{dt}{ds} = 0\,. \tag{1.5}$$

In contrast to the conventional phase-space Hamiltonian $H(\vec{q},\vec{p},t)$, where the time t plays the role of the independent variable, the extended phase-space Hamiltonian $\widetilde{H}(\vec{q},\vec{p},t,\mathcal{H})$ does *not* depend on its independent variable, s, hence describes formally an autonomous system. Of course, the function $\widetilde{H}$ must describe the dynamics of the given system *equivalently* to the initial Hamiltonian H. With the extended phase-space Hamiltonian $\widetilde{H}$, the variation integral (1.1) writes, analogously,

$$\delta\int_{s_1}^{s_2}\left[\sum_{i=1}^{n+1} p_i(s)\frac{dq_i(s)}{ds} - \widetilde{H}(q_1,\ldots,q_{n+1};p_1,\ldots,p_{n+1})\right]ds = 0\,, \tag{1.6}$$

hence, inserting $\widetilde{H}$ from Eq. (1.5)

$$\delta\int_{s_1}^{s_2}\left[\sum_{i=1}^{n} p_i\frac{dq_i}{ds} - \mathcal{H}\frac{dt}{ds} - \big(H(\vec{q},\vec{p},t) - \mathcal{H}\big)\frac{dt}{ds}\right]ds = \delta\int_{t_1}^{t_2}\left[\sum_{i=1}^{n} p_i\frac{dq_i}{dt} - H(\vec{q},\vec{p},t)\right]dt = 0\,.$$

Thus, with $\widetilde{H}$ given by Eq. (1.5), Hamilton's principle (1.6) in the extended phase space coincides with the conventional phase-space formulation of Eq. (1.1). In other words, the extension of the phase space meets the requirement to keep the description of the system's dynamics unchanged.

Similar to the case of Eq. (1.1), the variation integral (1.6) vanishes exactly if the canonical equations

$$\frac{dt}{ds} = -\frac{\partial\widetilde{H}}{\partial\mathcal{H}}\,, \qquad \frac{d\mathcal{H}}{ds} = \frac{\partial\widetilde{H}}{\partial t}\,, \qquad \frac{dq_i}{ds} = \frac{\partial\widetilde{H}}{\partial p_i}\,, \qquad \frac{dp_i}{ds} = -\frac{\partial\widetilde{H}}{\partial q_i}\,, \qquad i = 1,\ldots,n \tag{1.7}$$

hold for the "extended" Hamiltonian $\widetilde{H}$. In contrast to the time derivative of the original Hamiltonian H, the total s-derivative of $\widetilde{H}$ always vanishes identically by virtue of Eqs. (1.7)

$$\frac{d\widetilde{H}}{ds} \equiv \sum_{i=1}^{n}\left[\frac{\partial\widetilde{H}}{\partial q_i}\frac{dq_i}{ds} + \frac{\partial\widetilde{H}}{\partial p_i}\frac{dp_i}{ds}\right] + \frac{\partial\widetilde{H}}{\partial t}\frac{dt}{ds} + \frac{\partial\widetilde{H}}{\partial\mathcal{H}}\frac{d\mathcal{H}}{ds} \equiv 0\,.$$

Thus, $\widetilde{H}$ indeed describes an autonomous system in the $(2n+2)$-dimensional extended phase space. This means for the right hand side of Eq. (1.5)

$$\frac{d}{ds}\left[\big(H(\vec{q},\vec{p},t) - \mathcal{H}\big)\frac{dt}{ds}\right] = \big(H(\vec{q},\vec{p},t) - \mathcal{H}\big)\frac{d^2t}{ds^2} - \left(\frac{d\mathcal{H}}{ds} - \frac{dt}{ds}\frac{\partial H}{\partial t}\right)\frac{dt}{ds} \stackrel{!}{=} 0\,,$$

which is satisfied for

$$\frac{d\mathcal{H}}{ds} = \frac{dt}{ds}\frac{\partial H}{\partial t} \tag{1.8}$$

since the factor $(H(\vec{q},\vec{p},t)-\mathcal{H})$ vanishes by virtue of Eq. (1.4). We observe that Eq. (1.8) is consistent with the definition of $\mathcal{H}$ in Eq. (1.4) and can be regarded as the canonical equation for this extended phase-space variable. Calculating the partial derivatives of the Hamiltonian $\widetilde{H}$ on both sides of Eq. (1.5), we establish the relations of Eqs. (1.7) to the canonical equations (1.2) of the original Hamiltonian $H(\vec{q},\vec{p},t)$

$$\frac{\partial\widetilde{H}}{\partial p_i}=t'(s)\frac{\partial H}{\partial p_i}\,,\qquad\frac{\partial\widetilde{H}}{\partial q_i}=t'(s)\frac{\partial H}{\partial q_i}\,,\qquad\frac{\partial\widetilde{H}}{\partial t}=t'(s)\frac{\partial H}{\partial t}\,,\qquad\frac{\partial\widetilde{H}}{\partial\mathcal{H}}=-t'(s)\,. \tag{1.9}$$

Herein, $t'(s)=dt(s)/ds$ abbreviates the derivative of the canonical variable time $t(s)$ with respect to the independent variable s of the extended phase space. Obviously, a particular time parameterization $t=t(s)$ is not determined by $H(\vec{q},\vec{p},t)$. Indeed, inserting the last equation of (1.9) into the r.h.s. of the corresponding canonical equation (1.7) for $t(s)$, we simply get an identity satisfied by all functions $t(s)$. Defining $t(s)=s$ — as is often done in literature [10, 11] — is therefore a valid parameterization that trivially reduces the extended phase-space description to the conventional one. However, we will see in Sec. 1.1.2 in the context of canonical transformations in the extended phase space, that a non-trivial relation between t, the transformed time t', and s must be allowed in order to maintain the consistency of the concept of an extended phase space.

Summarizing, we may state that an explicitly time-dependent (non-autonomous) Hamiltonian system is formally rendered autonomous if described in the extended phase-space formalism. On the other hand, the two additional canonical equations do not provide additional information, and the "extended" set of canonical equations is strictly equivalent to the conventional one. This means that we do not encounter any advantage with regard to integrating the system's equations of motion by the formal addition of another degree of freedom. Nevertheless, as we shall see in Sec. 1.1.2, only the extended phase-space description offers the complete variety of possible canonical transformations of the system's canonical variables if the Hamiltonian system is explicitly time-dependent.

1.1.2 Canonical transformations in the extended phase space

The extended phase-space formulation has the benefit to allow for more general canonical transformations that also include a transformation of time

$$(\vec{q},\vec{p},t,\mathcal{H})\xrightarrow{\text{canon. transf.}}(\vec{q}\,',\vec{p}\,',t',\mathcal{H}')\,. \tag{1.10}$$

The transformation (1.10) is referred to as canonical if and only if Hamilton's variation principle (1.6) is maintained in the new (primed) set of canonical variables. The condition for an extended phase-space transformation (1.10) to be canonical can therefore be derived directly from the generalized Hamilton principle of Eq. (1.6)

$$\delta\int_{s_1}^{s_2}\left[\sum_{i=1}^{n}p_i\frac{dq_i}{ds}-\mathcal{H}\frac{dt}{ds}-\widetilde{H}\right]ds=\delta\int_{s_1}^{s_2}\left[\sum_{i=1}^{n}p_i'\frac{dq_i'}{ds}-\mathcal{H}'\frac{dt'}{ds}-\widetilde{H}'\right]ds=0\,.$$

This means that the integrands of the variation integrals may differ at most by a total differential of the extended phase-space variables q_i,t,q_i',t'. We demand the Hamiltonian to be maintained by virtue of the transformation (1.10)

$$\widetilde{H}(\vec{q},\vec{p},t,\mathcal{H})=\widetilde{H}'(\vec{q}\,',\vec{p}\,',t',\mathcal{H}')\,, \tag{1.11}$$

hence require the new Hamiltonian $\widetilde{H}'$ to represent as well a zero Hamiltonian of the form of Eq. (1.5). Then, the condition for the variation principle to be preserved becomes

$$\sum_{i=1}^{n}p_i dq_i-\mathcal{H}dt=\sum_{i=1}^{n}p_i'dq_i'-\mathcal{H}'dt'+dF_1(\vec{q},\vec{q}\,',t,t')\,. \tag{1.12}$$

The function $F_1(\vec{q}, \vec{q}\,', t, t')$ is commonly referred to as the "generating function" of the canonical transformation. In terms of its arguments, the total differential $dF_1(\vec{q}, \vec{q}\,', t, t')$ writes explicitly

$$dF_1 = \sum_{i=1}^{n} \left(\frac{\partial F_1}{\partial q_i} \, dq_i + \frac{\partial F_1}{\partial q_i'} \, dq_i' \right) + \frac{\partial F_1}{\partial t} \, dt + \frac{\partial F_1}{\partial t'} \, dt' \, . \tag{1.13}$$

Comparing Eq. (1.13) with Eq. (1.12), we obtain the transformation rules for the conjugate quantities p_i, $-\mathcal{H}$, p_i', and $-\mathcal{H}'$

$$p_i = \frac{\partial F_1}{\partial q_i} \, , \quad p_i' = -\frac{\partial F_1}{\partial q_i'} \, , \quad \mathcal{H} = -\frac{\partial F_1}{\partial t} \, , \quad \mathcal{H}' = \frac{\partial F_1}{\partial t'} \, .$$

With the help of the Legendre transformation

$$F_2(\vec{q}, \vec{p}\,', t, \mathcal{H}') = F_1(\vec{q}, \vec{q}\,', t, t') + \sum_{i=1}^{n} q_i' p_i' - t' \mathcal{H}' \, ,$$

the generating function may be expressed equivalently in terms of the old configuration space and the new momentum coordinates. If we compare the coefficients pertaining to the respective differentials dq_i, dp_i', dt, and $d\mathcal{H}'$, we find the following coordinate transformation rules to apply for each index $i = 1, \ldots, n$:

$$q_i' = \frac{\partial F_2}{\partial p_i'} \, , \quad p_i = \frac{\partial F_2}{\partial q_i} \, , \quad t' = -\frac{\partial F_2}{\partial \mathcal{H}'} \, , \quad \mathcal{H} = -\frac{\partial F_2}{\partial t} \, . \tag{1.14}$$

In Sec. 1.2.1, the rules (1.14) will be applied to transform a particular class of time-dependent Hamiltonians into time-independent ones.

Beforehand, Liouville's theorem [12] in the context of canonical transformations within the extended phase space will be discussed. We shall set up the condition for the generating function $F_2(\vec{q}, \vec{p}\,', t, \mathcal{H}')$ in order to define a canonical transformation that preserves the volume element of the non-extended phase space.

1.1.3 Liouville's theorem in the extended phase space

Performing a transformation of the actual canonical variables to a new set of "primed" variables

$$dq_1' \ldots dq_n' dp_1' \ldots dp_n' = D \, dq_1 \ldots dq_n dp_1 \ldots dp_n \, ,$$

the scaling factor D of the respective volume elements is given by the determinant of the related Jacobi matrix. Liouville's theorem now states that the phase-space volume element $d\Gamma$ is preserved if the transformation in question is canonical

$$d\Gamma = dq_1 \ldots dq_n dp_1 \ldots dp_n = dq_1' \ldots dq_n' dp_1' \ldots dp_n' \, .$$

This, in turn, implies that the determinant D of the Jacobi matrix associated with a canonical transformation is unity

$$D = \frac{\partial \left(q_1', \ldots, q_n', p_1', \ldots, p_n' \right)}{\partial \left(q_1, \ldots, q_n, p_1, \ldots, p_n \right)} = 1 \, . \tag{1.15}$$

As the system's time evolution itself constitutes a canonical transformation, this means more specifically that the volume element $d\Gamma$ provides a constant of motion. The proof of Eq. (1.15) is straightforwardly worked out [12] making use of the fact that a generating function F_2 necessarily exists if the transformation is canonical.

We will now investigate the condition for the volume element of the extended phase space $dq_1 \dots dq_{n+1} dp_1 \dots dp_{n+1}$ to be conserved as well. First of all, we note that the value of the related determinant $\widetilde{D}$ cannot depend on the numbering of the canonical variables[1]

$$\widetilde{D} = \frac{\partial \left(q_1', \dots, q_n', p_1', \dots, p_n', t', -\mathcal{H}'\right)}{\partial \left(q_1, \dots, q_n, p_1, \dots p_n, t, -\mathcal{H}\right)} \,.$$

Furthermore, the Jacobian $\widetilde{D}$ can be expressed equivalently as the product of the determinants

$$\widetilde{D} = \left.\frac{\partial \left(q_1', \dots, q_n', p_1', \dots, p_n'\right)}{\partial \left(q_1, \dots, q_n, p_1, \dots p_n\right)}\right|_{t,\mathcal{H}=\text{const.}} \times \quad \left.\frac{\partial \left(t', -\mathcal{H}'\right)}{\partial \left(t, -\mathcal{H}\right)}\right|_{\vec{q},\vec{p}=\text{const.}} \,.$$

We conclude that Liouville's theorem applies as well for the extended phase space exactly if the right hand side factor is unity

$$\left.\frac{\partial \left(t', -\mathcal{H}'\right)}{\partial \left(t, -\mathcal{H}\right)}\right|_{\vec{q},\vec{p}=\text{const.}} = \frac{\partial t'}{\partial t}\frac{\partial \mathcal{H}'}{\partial \mathcal{H}} - \frac{\partial t'}{\partial \mathcal{H}}\frac{\partial \mathcal{H}'}{\partial t} = 1 \,. \tag{1.16}$$

A necessary and sufficient condition for a transformation (1.10) to be canonical is that any pair of canonical conjugate variables must satisfy the Poisson bracket condition

$$\left[p_i', q_j'\right] = \sum_{k=1}^{n+1} \left(\frac{\partial p_i'}{\partial p_k}\frac{\partial q_j'}{\partial q_k} - \frac{\partial p_i'}{\partial q_k}\frac{\partial q_j'}{\partial p_k} \right) = \delta_{ij} \,.$$

For $i = j = n + 1$, i.e. for the pair of conjugate coordinates $(t', -\mathcal{H}')$, this means

$$\left[-\mathcal{H}', t'\right] = \sum_{k=1}^{n} \left(-\frac{\partial \mathcal{H}'}{\partial p_k}\frac{\partial t'}{\partial q_k} + \frac{\partial \mathcal{H}'}{\partial q_k}\frac{\partial t'}{\partial p_k} \right) + \frac{\partial \mathcal{H}'}{\partial \mathcal{H}}\frac{\partial t'}{\partial t} - \frac{\partial \mathcal{H}'}{\partial t}\frac{\partial t'}{\partial \mathcal{H}} = 1 \,.$$

Condition (1.16) thus coincides with the requirement that

$$\sum_{k=1}^{n} \left(\frac{\partial \mathcal{H}'}{\partial q_k}\frac{\partial t'}{\partial p_k} - \frac{\partial \mathcal{H}'}{\partial p_k}\frac{\partial t'}{\partial q_k} \right) = 0 \,,$$

which is satisfied if the transformed time t' does not depend on the individual particle coordinates

$$\frac{\partial t'}{\partial p_i} = \frac{\partial t'}{\partial q_i} = 0 \,, \qquad i = 1, \dots, n \,.$$

This means that t' must be the same for all particles i. Liouville's theorem thus holds for canonical transformations in the extended phase space exactly if the variable "time" remains a global quantity that parameterizes equally the motion of all particles. With Eq. (1.14), this means for a function $F_2(\vec{q}, \vec{p}\,', t, \mathcal{H}')$ that generates an extended phase-space canonical transformation

$$\frac{\partial}{\partial p_i}\left(\frac{\partial F_2}{\partial \mathcal{H}'}\right) = \frac{\partial}{\partial q_i}\left(\frac{\partial F_2}{\partial \mathcal{H}'}\right) = 0 \,, \qquad i = 1, \dots, n \,.$$

The generating function F_2 for the canonical transformation that will be carried out for a class of Hamiltonian systems in the next section will have this property.

[1]This reordering of the determinant's canonical variables implies both n interchanges of rows and n interchanges of columns, hence no change of sign of $\widetilde{D}$.

1.2 Invariants for time-dependent Hamiltonian systems

1.2.1 Invariant derived from a canonical transformation

We will show in the following that a fairly general class of explicitly time-dependent Hamiltonians H can be mapped by a finite extended phase-space transformation onto a Hamiltonian H' that no longer depends on time explicitly [13]. The new Hamiltonian H' then describes an autonomous system — hence embodies an invariant $I \equiv H'$ that represents the system's conserved total energy. As this transformation is unique, we may conceive the transformed system described by H' as the *equivalent* autonomous system of H.

The class of Hamiltonians to be considered now describes n-degree-of-freedom systems of particles that move in explicitly time-dependent potentials $V(\vec{q},t)$ under the action of time-dependent damping forces proportional to the velocity

$$H = \tfrac{1}{2} e^{-F(t)} \sum_{i=1}^{n} p_i^2 + e^{F(t)} V(\vec{q},t) \quad \text{with} \quad F(t) = \int_{t_0}^{t} f(\tau)\, d\tau \,. \tag{1.17}$$

It provides the canonical equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = p_i\, e^{-F(t)} \,, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} = -\frac{\partial V}{\partial q_i} e^{F(t)} \,, \tag{1.18}$$

hence the equation of motion

$$\ddot{q}_i + f(t)\,\dot{q}_i + \frac{\partial V(\vec{q},t)}{\partial q_i} = 0 \,. \tag{1.18a}$$

The Hamiltonian (1.17) will be transformed by means of a canonical transformation into the new Hamiltonian

$$H'(\vec{q}\,',\vec{p}\,') = \tfrac{1}{2} \sum_{i=1}^{n} p_i'^{\,2} + V'(\vec{q}\,') \,, \tag{1.19}$$

which is supposed to be independent of time explicitly. The canonical transformation in the extended phase space be generated by

$$F_2(\vec{q},\vec{p}\,',t,\mathcal{H}') = \phi_2(\vec{q},\vec{p}\,',t) - \mathcal{H}' \int_{t_0}^{t} \frac{d\tau}{\xi(\tau)} \,. \tag{1.20}$$

The function $\phi_2(\vec{q},\vec{p}\,',t)$ contained herein be defined as the following generating function in the usual (non-extended) phase space

$$\phi_2(\vec{q},\vec{p}\,',t) = \sqrt{\frac{e^{F(t)}}{\xi(t)}} \sum_{i=1}^{n} q_i\, p_i' + \tfrac{1}{4} e^{F(t)} \left(\frac{\dot{\xi}(t)}{\xi(t)} - f(t) \right) \sum_{i=1}^{n} q_i^2 \,. \tag{1.21}$$

For the moment, $\xi(t)$ may be regarded as an arbitrary differentiable function of time only. Working out the transformation rules (1.14) for the specific generating function F_2, as defined by (1.20), we find the following time-dependent linear transformation between the old $\{q_i, p_i\}$ and the new set of coordinates $\{q_i', p_i'\}$

$$\begin{pmatrix} q_i \\ p_i \end{pmatrix} = \begin{pmatrix} \sqrt{\xi(t)/e^{F(t)}} & 0 \\ \tfrac{1}{2}\big(\dot{\xi} - \xi f\big) \sqrt{e^{F(t)}/\xi(t)} & \sqrt{e^{F(t)}/\xi(t)} \end{pmatrix} \begin{pmatrix} q_i' \\ p_i' \end{pmatrix} . \tag{1.22}$$

Furthermore, the transformations of time t and Hamiltonian H are given by

$$t' = -\frac{\partial F_2}{\partial \mathcal{H}'} = \int_{t_0}^{t} \frac{d\tau}{\xi(\tau)}\,, \qquad \mathcal{H} = -\frac{\partial F_2}{\partial t} = -\frac{\partial \phi_2}{\partial t} + \frac{\mathcal{H}'}{\xi(t)}\,. \tag{1.23}$$

We easily verify that the canonical transformation within the scope of the extended phase space, defined by Eqs. (1.22) and (1.23), satisfies the fundamental Poisson brackets

$$\left[p_i', q_j'\right]_{\vec{p},\vec{q}} = \delta_{ij}\,, \qquad \left[-\mathcal{H}', t'\right]_{-\mathcal{H},t} = 1\,.$$

From (1.23), the new Hamiltonian H' follows as the projection to the conventional phase space according to Eq. (1.4)

$$H'\big|_{t'} = \xi(t)\left(H + \frac{\partial \phi_2}{\partial t}\right)\,. \tag{1.24}$$

The transformed Hamiltonian H' of Eq. (1.24) is obtained in the desired form of Eq. (1.19) if the old Hamiltonian H as well as the partial time derivative of Eq. (1.21) are expressed in terms of the new (primed) coordinates. Explicitly, the effective potential $V'(\vec{q}\,')$ of the transformed system evaluates to

$$V'(\vec{q}\,') = \tfrac{1}{4}\Big[\ddot{\xi}\xi - \tfrac{1}{2}\dot{\xi}^2 - \xi^2\big(\dot{f} + \tfrac{1}{2}f^2\big)\Big]\sum_{i=1}^{n} q_i'^{\,2} + \xi\, e^{F(t)}\, V\big(\sqrt{\xi\, e^{-F}}\,\vec{q}\,', t\big)\,. \tag{1.25}$$

The new potential V' consists of two components, namely, a term related to the original potential V, and an additional quadratic potential that describes the linear forces of inertia occurring due to the time-dependent linear transformation (1.22) to a new frame of reference.

The required property of the new Hamiltonian (1.19) to describe an autonomous system is met if and only if the new potential $V'(\vec{q}\,')$ does not depend on time t explicitly. This means that the initially arbitrary function $\xi(t)$ — defined in the generating function (1.20) — is now tailored to eliminate an explicit time-dependence of V' at the location $\vec{q}\,'$. In order to set up the appropriate conditional equation for $\xi(t)$, we calculate the partial time derivative of Eq. (1.25)

$$\begin{aligned}\frac{\partial V'(\vec{q}\,')}{\partial t'} = \tfrac{1}{4}\xi e^{F}\Bigg\{&\Big(\dddot{\xi} - 2\dot{\xi}\dot{f} - \xi\ddot{f} - \dot{\xi}f^2 - \xi f\dot{f}\Big)\,\xi\, e^{-F}\sum_{i=1}^{n} q_i'^{\,2}\\ &+4\dot{\xi}\left(V + \tfrac{1}{2}\sum_{i=1}^{n} q_i'\frac{\partial V}{\partial q_i'}\right) + 4\xi\left(\frac{\partial V}{\partial t} + fV - \tfrac{1}{2}f\sum_{i=1}^{n} q_i'\frac{\partial V}{\partial q_i'}\right)\Bigg\} = 0\,. \end{aligned}\tag{1.26}$$

Inserting the transformation rules that follow from (1.22)

$$q_i'^{\,2} = \frac{e^F}{\xi}q_i^2\,, \qquad q_i'\frac{\partial V}{\partial q_i'} = q_i\frac{\partial V}{\partial q_i}\,,$$

Equation (1.26) leads to the following linear differential equation for $\xi(t)$

$$\begin{aligned}\dddot{\xi}\sum_{i=1}^{n} q_i^2 + 4\dot{\xi}&\left[V(\vec{q},t) + \tfrac{1}{2}\sum_{i=1}^{n} q_i\frac{\partial V}{\partial q_i} - \tfrac{1}{2}\left(\dot{f} + \tfrac{1}{2}f^2\right)\sum_{i=1}^{n} q_i^2\right]\\ &+ 4\xi\left[\frac{\partial V}{\partial t} + f\left(V(\vec{q},t) - \tfrac{1}{2}\sum_{i=1}^{n} q_i\frac{\partial V}{\partial q_i}\right) - \tfrac{1}{4}\left(\ddot{f} + f\dot{f}\right)\sum_{i=1}^{n} q_i^2\right] = 0\,. \end{aligned}\tag{1.27}$$

With $\xi(t)$ a solution of Eq. (1.27), we thus have

$$\frac{\partial V'(\vec{q}\,')}{\partial t'} = 0\,,$$

which means that the Hamiltonian

$$H'(\vec{q}\,',\vec{p}\,') = \tfrac{1}{2}\sum_{i=1}^{n} p_i'^{\,2} + V'(\vec{q}\,') = I \tag{1.28}$$

does not depend on time explicitly, hence constitutes a constant of motion.

The Hamiltonian H' of Eq. (1.28) may be expressed as well in terms of the old coordinates $\{q_i, p_i\}$ which finally provides the invariant I of our time-dependent system (1.17)

$$I = \xi\, H - \tfrac{1}{2}\Big(\dot{\xi} - \xi\, f\Big)\sum_{i=1}^{n} q_i\, p_i + \tfrac{1}{4}e^{F(t)}\,\Big(\ddot{\xi} - \dot{\xi} f - \xi\dot{f}\Big)\sum_{i=1}^{n} q_i^2\,. \tag{1.29}$$

We may directly prove that the quantity I of Eq. (1.29) is indeed a constant of motion[2] by showing that the Poisson bracket $[I, H]$ together with the auxiliary equation (1.27) yields the partial time derivative of I

$$\frac{dI}{dt} = 0 \qquad \Longleftrightarrow \qquad \frac{\partial I}{\partial t} = [I, H]\ .$$

The effect of the finite canonical transformation generated by (1.20) can be summarized as a transfer of the time-dependence from the original Hamiltonian $H(\vec{q},\vec{p},t)$ into the time-dependence of the frame of reference in the extended phase space of the new Hamiltonian $H'(\vec{q}\,',\vec{p}\,')$. In other words, the autonomous system's Hamiltonian H' is *canonically equivalent* to the initial time-dependent Hamiltonian system H.

For $\xi(t) > 0$, the Hamiltonian H' represents a real physical system. Because of the uniqueness of the transformation rules (1.22) and (1.23), the Hamiltonian system H' may then be conceived as the autonomous system that is *physically equivalent* to the initial system described by H.

The instants of time t with $\xi(t) = 0$ mark the singular points where this transformation does not exist. For time intervals with $\xi(t) < 0$, the elements of coordinate transformation matrix (1.22) become imaginary, and — according to (1.23) — the flow of the transformed time t' with respect to t becomes negative. Under these circumstances, the transformed system does not possess a physical meaning anymore, which means that the equivalent autonomous system ceases to exist as a physical system. In other words, the particle motion within the time-dependent non-linear system can no longer be expressed as the linearly transformed motion within an autonomous system.

On the other hand, the invariant I in the representation of Eq. (1.29) exists for all $\xi(t)$ that are solutions of Eq. (1.27), including the regions with $\xi(t) \le 0$. We may regard (1.29) as an implicit function $I = I(\vec{q},\vec{p},t)$ of the phase-space coordinates, visualized as a time-varying $(2n-1)$-dimensional surface in the $2n$-dimensional phase space.

To end this section, we finally note that a canonical transformation that maps an explicitly time-dependent Hamiltonian H into a time-independent H' can equivalently be formulated in the conventional (non-extended) phase space. Presenting a two-step linear canonical transformation, this has been demonstrated for the damped *linear* oscillator by Leach [14]. A similar transformation that is followed by a rescaling of time [15] has been shown capable to work out invariants for more general cases of time-dependent *non-linear* Hamiltonian systems.

1.2.2 Review of Noether's theorem

Noether's theorem [2, 16, 17] relates the conserved quantities of a Lagrangian system $L(\vec{q},\dot{\vec{q}},t)$ to the one-parameter groups of infinitesimal point transformations that leave the Lagrange action $L\,dt$ invariant. We now work out this theorem in explicit form, hence isolate a conserved quantity of a Lagrangian system that is subject to an infinitesimal point transformation. By an

[2] Some authors refer to phase-space invariants that depend on time explicitly as "integrals of motion", reserving the notation "constants of motion" for invariants that do *not* depend on time explicitly.

infinitesimal point transformation we mean those transformations that map "points" into "points": $(\vec{q},t) \mapsto (\vec{q}',t')$, the primes indicating the transformed quantities. We hereby determine uniquely the mapping of the time derivative of $\vec{q}$, i.e. the transformation $\dot{\vec{q}} \mapsto \dot{\vec{q}}'$. A point transformation that depends on an infinitesimal parameter ε may be defined formally by

$$t' = t + \delta t + \ldots = t + \varepsilon\xi(t) + \ldots \tag{1.30a}$$
$$q_i' = q_i + \delta q_i + \ldots = q_i + \varepsilon\eta_i(q_i,t) + \ldots \tag{1.30b}$$
$$\dot{q}_i' = \dot{q}_i + \delta\dot{q}_i + \ldots \tag{1.30c}$$

with

$$\xi(t) = \left.\frac{\partial t'}{\partial\varepsilon}\right|_{\varepsilon=0}, \qquad \eta_i(q_i,t) = \left.\frac{\partial q_i'}{\partial\varepsilon}\right|_{\varepsilon=0}.$$

In order to express a given Lagrange function $L(\vec{q},\dot{\vec{q}},t)$ in terms of the primed variables, we must know the transformation of the $\dot{q}_i$ for the infinitesimal point transformation defined by Eqs. (1.30a) and (1.30b). We note that $\delta\dot{q}_i$ in Eq. (1.30c) does *not* stand for the time derivative of δq_i since both the coordinates q_i as well as the time t are subject to the infinitesimal transformation (1.30). The quantity $\delta\dot{q}_i$ follows from the consideration that $\dot{q}_i'$ is given by the derivative of the transformed coordinate q_i' with respect to the transformed time t'. According to the transformation rules (1.30), we thus find [18]

$$\dot{q}_i' = \frac{dq_i'}{dt'} = \frac{dq_i + \varepsilon d\eta_i}{dt + \varepsilon d\xi} = \frac{\dot{q}_i + \varepsilon\dot{\eta}_i}{1 + \varepsilon\dot{\xi}} = \dot{q}_i + \varepsilon\dot{\eta}_i - \varepsilon\dot{\xi}\dot{q}_i + \mathcal{O}(\varepsilon^2),$$

which means that the first order variation $\delta\dot{q}_i$ is given by

$$\delta\dot{q}_i = \varepsilon\big(\dot{\eta}_i - \dot{\xi}\dot{q}_i\big). \tag{1.31}$$

We now consider the particular subset of infinitesimal point transformations (1.30) that leave the Lagrange action Ldt invariant

$$L\big(\vec{q},\dot{\vec{q}},t\big)\,dt \stackrel{!}{=} L'\big(\vec{q}',\dot{\vec{q}}',t'\big)\,dt'. \tag{1.32}$$

By virtue of Hamilton's principle, the system's equations of motion follow from the variation of the action integral: $\delta\int Ldt = 0$. This implies that the particular symmetry transformations that leave the Lagrange action Ldt invariant sustain the form of the equations of motion.

The *functional* relation between L' and L may be expressed introducing an auxiliary function $\dot{f}_0(\vec{q},t)$

$$L'\big(\vec{q}',\dot{\vec{q}}',t'\big) = L + \delta L + \cdots = L\big(\vec{q}',\dot{\vec{q}}',t'\big) - \varepsilon\dot{f}_0(\vec{q},t) + \mathcal{O}(\varepsilon^2). \tag{1.30d}$$

For the relation (1.30d) to hold in general it is necessary and sufficient [16] that $f_0(\vec{q},t)$ depends on $\vec{q}$ and t only since, according to Eqs. (1.30c) and (1.31), the transformation $\dot{\vec{q}} \mapsto \dot{\vec{q}}'$ is uniquely determined by $\vec{q} \mapsto \vec{q}'$ and $t \mapsto t'$. Our task is now to determine $\dot{f}_0(\vec{q},t)$ for an infinitesimal point transformation (1.30) that fulfills Eq. (1.32). Inserting Eq. (1.30d) into the condition for the invariant Lagrange action (1.32), we get to first order in ε

$$L\big(\vec{q},\,\dot{\vec{q}},t\big)\,dt = L\big(\vec{q}',\dot{\vec{q}}',t'\big)\,dt' - \varepsilon\dot{f}_0(\vec{q},t)\,dt. \tag{1.33}$$

On the other hand, we may express $L\big(\vec{q}',\dot{\vec{q}}',t'\big)$ in terms of a truncated Taylor expansion of $L\big(\vec{q},\dot{\vec{q}},t\big)$

$$L\big(\vec{q}',\dot{\vec{q}}',t'\big)\,dt' = \left(L\big(\vec{q},\dot{\vec{q}},t\big) + \frac{\partial L}{\partial t}\delta t + \sum_{i=1}^{n}\left[\frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial\dot{q}_i}\delta\dot{q}_i\right]\right)dt'$$

With $dt' = (1 + \varepsilon\dot{\xi})\, dt$ and the above expressions for δt, δq_i, and $\delta\dot{q}_i$ this means to first order in ε

$$L\big(\vec{q}', \dot{\vec{q}}', t'\big)\, dt' = \left(L\big(\vec{q}, \dot{\vec{q}}, t\big) \big(1 + \varepsilon\dot{\xi}\big) + \frac{\partial L}{\partial t}\varepsilon\xi + \varepsilon \sum_{i=1}^{n} \left[\frac{\partial L}{\partial q_i}\eta_i + \frac{\partial L}{\partial \dot{q}_i}\big(\dot{\eta}_i - \dot{q}_i\dot{\xi}\big) \right] \right) dt\,. \quad (1.34)$$

Combining Eqs. (1.33) and (1.34), we obtain the differential equation for $f_0(\vec{q}, t)$

$$\dot{f}_0(\vec{q}, t) - \dot{\xi}\, L(\vec{q}, \dot{\vec{q}}, t) - \xi\, \frac{\partial L}{\partial t} - \sum_{i=1}^{n} \left[\eta_i \frac{\partial L}{\partial q_i} + \big(\dot{\eta}_i - \dot{q}_i\dot{\xi}\big) \frac{\partial L}{\partial \dot{q}_i} \right] = 0\,. \quad (1.35)$$

We may regard Eq. (1.35) as a condition for the yet unspecified functions $\xi(\vec{q}, t)$ and $\eta_i(\vec{q}, t)$. Only those point transformations (1.30) whose constituents ξ and η_i satisfy Eq. (1.35) maintain the Lagrange action Ldt for the given Lagrangian $L(\vec{q}, \dot{\vec{q}}, t)$.

The terms of Eq. (1.35) can directly be split into a total time derivative and a sum containing the Euler-Lagrange equations of motion

$$\frac{d}{dt} \left[f_0(\vec{q}, t) - \xi\, L + \sum_{i=1}^{n} (\xi\dot{q}_i - \eta_i) \frac{\partial L}{\partial \dot{q}_i} \right] + \sum_{i=1}^{n} (\xi\dot{q}_i - \eta_i) \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} \right) = 0\,. \quad (1.36)$$

Along the system trajectory $\big(\vec{q}(t), \dot{\vec{q}}(t)\big)$ given by the solutions of the Euler-Lagrange equations

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = 0\,, \qquad i = 1, \ldots, n\,, \quad (1.37)$$

the corresponding terms of Eq. (1.36) vanish. This means that the time integral I of the remaining terms

$$I = \sum_{i=1}^{n} (\xi\dot{q}_i - \eta_i) \frac{\partial L}{\partial \dot{q}_i} - \xi\, L + f_0(\vec{q}, t) \quad (1.38)$$

constitutes a conserved quantity, i.e. a constant of motion for the Lagrange system $L(\vec{q},\dot{\vec{q}},t)$. The invariant given by Eq. (1.38) together with the differential equation (1.35) for $f_0(\vec{q}, t)$ is commonly referred to as Noether's theorem. The invariant of Eq. (1.38) does not contain unknown time integrals as long as the "gauge" function $\dot{f}_0(\vec{q}, t)$ — defined in Eq. (1.30d) — constitutes a total time derivative. Starting from the initial condition $(\vec{q}(t_0), \dot{\vec{q}}(t_0))$, the system's state $(\vec{q}(t), \dot{\vec{q}}(t))$ is uniquely determined by the equations of motion (1.37) — which in turn follow from Hamilton's principle $\delta \int L dt = 0$. Writing the variation $\delta \int L' dt' = 0$ of the infinitesimally transformed system in terms of the original coordinates, we obtain *in addition* to the equations of motion (1.37) the quantity I that is conserved by virtue of the symmetry transformation (1.30). Thus, the requirement $\delta \int L' dt' = 0$ may be seen a generalization of Hamilton's principle that yields both the equations of motion *and* a phase space symmetry relation embodied in the invariant I. In general, the equation (1.35) for $f_0(\vec{q}, t)$ depends on $\vec{q}(t)$, hence on the solutions of the equations of motion (1.37). Equation (1.35) together with the equations of motion (1.37) thus represents an extended coupled set of differential equations whose solution yields a symmetry relation in addition to the evolution of the system trajectory.

We will show in the following section that the invariant (1.29) for the Hamiltonian system (1.17) can equivalently be derived on the basis of Noether's theorem in the context of the Lagrange formalism.

1.2.3 Invariant derived from Noether's theorem

The particular Lagrangian, whose Euler-Lagrange equations (1.37) lead to the equations of motion (1.18a) follows from the Legendre transformation

$$L(\vec{q}, \dot{\vec{q}}, t) = \sum_{i=1}^{n} p_i\, \dot{q}_i - H(\vec{q}, \vec{p}, t)\,, \qquad \dot{q}_i = \frac{\partial H}{\partial p_i} = e^{-F} p_i = e^{-F} \frac{\partial L}{\partial \dot{q}_i} \quad (1.39)$$

as

$$L(\vec{q},\dot{\vec{q}},t)=\left(\sum_{i=1}^{n}\tfrac{1}{2}\dot{q}_i^2-V(\vec{q},t)\right)e^{F(t)}\quad\text{with}\quad F(t)=\int_{t_0}^{t}f(\tau)d\tau\,. \tag{1.40}$$

Inserting the Lagrangian (1.40) and its partial derivatives into Eq. (1.35), we get

$$\begin{aligned}\frac{\partial f_0}{\partial t}+\xi e^F\frac{\partial V}{\partial t}+\sum_i\dot{q}_i\frac{\partial f_0}{\partial q_i}-e^F\Big(\dot{\xi}+\xi f\Big)\Big(\sum_i\tfrac{1}{2}\dot{q}_i^2-V\Big)&\\ -e^F\sum_i\left(\dot{q}_i\frac{\partial\eta_i}{\partial t}+\dot{q}_i^2\frac{\partial\eta_i}{\partial q_i}-\dot{q}_i^2\dot{\xi}-\eta_i\frac{\partial V}{\partial q_i}\right)&=0\,.\end{aligned} \tag{1.41}$$

Equation (1.41) must hold independently of the specific phase-space location of each individual particle i. Therefore, the coefficients pertaining to the velocity powers must vanish separately for each index i. This means for the terms proportional to $\dot{q}_i^2$

$$\frac{\partial\eta_i}{\partial q_i}=\tfrac{1}{2}\dot{\xi}-\tfrac{1}{2}\xi f\,,$$

which can be integrated to give

$$\eta_i(q_i,t)=\tfrac{1}{2}\Big[\dot{\xi}(t)-\xi(t)f(t)\Big]q_i+\psi_i(t)\,. \tag{1.42}$$

The terms of Eq. (1.41) that are linear in $\dot{q}_i$ vanish if the condition

$$\frac{\partial f_0}{\partial q_i}-e^F\frac{\partial\eta_i}{\partial t}=0 \tag{1.43}$$

is fulfilled for each i. Inserting the partial time derivative of Eq. (1.42) into Eq. (1.43), this gives

$$\frac{\partial f_0}{\partial q_i}=\tfrac{1}{2}e^F\left(\ddot{\xi}-\dot{\xi}f-\xi\dot{f}\right)q_i+e^F\dot{\psi}_i(t)$$

which can again be directly integrated to obtain $f_0(\vec{q},t)$

$$f_0(\vec{q},t)=e^{F(t)}\Big[\tfrac{1}{4}\big(\ddot{\xi}-\dot{\xi}f-\xi\dot{f}\big)\sum_{i=1}^{n}q_i^2+\sum_{i=1}^{n}\dot{\psi}_iq_i\Big]\,. \tag{1.44}$$

The remaining terms of Eq. (1.41) that do not depend on $\dot{q}_i$ sum up to

$$\frac{\partial f_0}{\partial t}+e^{F(t)}\left[\sum_{i=1}^{n}\eta_i\frac{\partial V}{\partial q_i}+\xi\left(\frac{\partial V}{\partial t}+f(t)V\right)+\dot{\xi}V\right]=0\,. \tag{1.45}$$

Inserting (1.42) and the partial time derivative of (1.44) into (1.45), we get the third-order differential equation for $\xi(t)$ of Eq. (1.27), together with a set of conditional equations for the functions $\psi_i(t)$ which must vanish separately for each index i

$$\ddot{\psi}_i\,q_i-\psi_i\,\ddot{q}_i+f(t)\big(\dot{\psi}_i\,q_i-\psi_i\,\dot{q}_i\big)=0\,. \tag{1.46}$$

The particular Noether invariant I for the Lagrange system (1.40)

$$\begin{aligned}I=e^{F(t)}\bigg\{\xi\Big[\sum_i\tfrac{1}{2}\dot{q}_i^2+V(\vec{q},t)\Big]-\tfrac{1}{2}\Big(\dot{\xi}-\xi\,f\Big)\sum_i q_i\,\dot{q}_i&\\ +\tfrac{1}{4}\Big(\ddot{\xi}-\dot{\xi}f-\xi\dot{f}\Big)\sum_i q_i^2+\sum_i\left(\dot{\psi}_iq_i-\psi_i\dot{q}_i\right)\bigg\}&\end{aligned} \tag{1.47}$$

is finally obtained inserting Eqs. (1.40), (1.42), and (1.44) into the general form (1.38) of the Noether invariant. Obviously, the ξ-dependent part of I agrees with the invariant (1.29) obtained from the canonical transformation of Sec. 1.2.1. In agreement with Eq. (1.46), the ψ-dependent sum of Eq. (1.47) constitutes a separate invariant. We conclude that the extended phase-space canonical transformation (1.20) of the Hamiltonian (1.17) is consistent with the infinitesimal symmetry transformation (1.30) of the equivalent Lagrangian.

1.2.4 Noether's theorem in the Hamiltonian formalism

From the definition (1.39) of the Legendre transformation that maps a given Lagrangian $L(\vec{q}, \dot{\vec{q}}, t)$ into the corresponding Hamiltonian $H(\vec{q}, \vec{p}, t)$, one finds the relations

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \qquad \dot{p}_i = \frac{\partial L}{\partial q_i}, \qquad \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t} = -\frac{dH}{dt}. \tag{1.48}$$

Applying these transformation rules for the transition from a Lagrangian description of a dynamical system to a Hamiltonian description to the Noether invariant of Eq. (1.38), one immediately gets

$$I = \sum_i^n \left[\xi \dot{q}_i - \eta_i(q_i, t)\right] p_i - \xi \sum_{i=1}^n p_i\, \dot{q}_i + \xi\, H + f_0(\vec{q}, t)\,,$$

which simplifies to the Hamiltonian formulation of Noether's theorem

$$I = \xi(t)\, H(\vec{q}, \vec{p}, t) - \sum_{i=1}^n \eta_i(q_i, t)\, p_i + f_0(\vec{q}, t)\,. \tag{1.49}$$

The conditional equation for $f_0(\vec{q},t)$, given by Eq. (1.35), translates according to Eqs. (1.48)

$$\dot{f}_0(\vec{q}, t) = -\xi\, \frac{dH}{dt} - \dot{\xi}\, H + \sum_{i=1}^n \dot{\xi} p_i\, \dot{q}_i + \sum_{i=1}^n \left(\eta_i \dot{p}_i + \dot{\eta}_i p_i - \dot{\xi} p_i\, \dot{q}_i\right)\,,$$

which can be written in the form of a total time derivative

$$\frac{d}{dt}\left[\xi(t)\, H(\vec{q}, \vec{p}, t) - \sum_{i=1}^n \eta_i(q_i, t)\, p_i + f_0(\vec{q}, t)\right] = 0\,.$$

In the Hamiltonian formulation, the conditional equation (1.35) thus appears as the requirement that the total time derivative of the invariant (1.49) vanishes

$$\frac{dI}{dt} \stackrel{!}{=} 0\,. \tag{1.50}$$

With the Hamiltonian H of Eq. (1.17), the form (1.49) of the Noether invariant is compatible with the Ansatz function used earlier by Lewis and Leach [19] with quadratic and linear terms in the canonical momentum. We thereby observe that this Ansatz approach to work out an invariant is equivalent to the strategy based on Noether's theorem.

The particular form of the invariant (1.29) for the Hamiltonian (1.17) may be derived equivalently on the basis of Eq. (1.50) with I given by Eq. (1.49). To this end, we must calculate the total time derivative of Eq. (1.49), insert the particular canonical equations (1.18), and equate to zero separately the sums proportional to p_i^2, p_i^1, and p_i^0 — similar to the procedure pursued in the approach based on Noether's theorem. We hereby observe a complete analogy deriving the invariant I for the Lagrangian (1.40) on the basis of Noether's theorem of Eqs. (1.38) and (1.35) with the approach of Eqs. (1.49) and (1.50) for the Hamiltonian (1.17). This shows that the invariant I of Eq. (1.49) provides indeed the Hamiltonian formulation of the Noether invariant (1.38).

1.2.5 System of variational equations

The system of canonical equations (1.2) may be written equivalently in the form of a set of $2n$ nonlinear first order differential equations

$$\frac{d}{dt}\,\vec{x} = \vec{f}(\vec{x}, t)\,, \qquad \dot{x}_i = f_i(x_1, \ldots, x_{2n}, t)\,, \qquad i = 1, \ldots, 2n\,, \tag{1.51}$$

with $\vec{x} = (q_1, p_1, \dots, q_n, p_n)^T$ the $2n$-dimensional vector of pairs of particle positions and the associated canonical momenta. Let $\delta\vec{x}$ denote the infinitesimal quantity that describes a neighboring solution of the system (1.51)

$$\frac{d}{dt}\left(\vec{x} + \delta\vec{x}\right) = \vec{f}\left(\vec{x} + \delta\vec{x}, t\right) .$$

We may now set up the system of variational equations in the form of a Taylor expansion

$$\frac{d}{dt}\left(x_i + \delta x_i\right) = f_i\left(\vec{x}, t\right) + \sum_{j=1}^{2n} \frac{\partial f_i}{\partial x_j} \delta x_j + \dots , \qquad i = 1, \dots, 2n .$$

As the δx_i are infinitesimal quantities by definition, we may truncate the Taylor series after its linear term to obtain a linear system of differential equations for the δx_i

$$\frac{d}{dt}\,\delta x_i = \sum_{j=1}^{2n} \frac{\partial f_i}{\partial x_j} \delta x_j , \qquad i = 1, \dots, 2n . \tag{1.52}$$

Together with the system of equations of motion (1.51), the linear system (1.52) of $2n$ first order equation determines both the evolution of the system trajectory $\vec{x}(t)$ and its related vector $\delta\vec{x}(t)$ that determines the stability of small perturbations.

With respect to the “extended” system description discussed in the context of Noether’s theorem in Sec. 1.2.2, we may regard the third order auxiliary equation (1.27) as an additional set of three first order equations of motion for $\xi(t)$, $\dot{\xi}(t)$, and $\ddot{\xi}(t)$. Identifying $x_{2n+1} \equiv \xi$, $x_{2n+2} \equiv \dot{\xi}$, and $x_{2n+3} \equiv \ddot{\xi}$, the “extended” set of equations of motion may be written in accordance to (1.51)

$$\dot{x}_i = f_i(x_1, \dots, x_{2n+3}, t) , \qquad i = 1, \dots, 2n + 3 . \tag{1.53}$$

Similarly, the extended set of variational equations is given by

$$\frac{d}{dt}\,\delta x_i = \sum_{j=1}^{2n+3} \frac{\partial f_i}{\partial x_j} \delta x_j , \qquad i = 1, \dots, 2n + 3 , \tag{1.54}$$

with $\delta x_{2n+1} \equiv \delta\xi$, $\delta x_{2n+2} \equiv \delta\dot{\xi}$, and $\delta x_{2n+1} \equiv \delta\ddot{\xi}$ the variations of the auxiliary function $\xi(t)$ and its derivatives due to an infinitesimal variation $\delta\vec{x}(t)$ of the system trajectory $\vec{x}(t)$.

1.2.6 Invariant for the system of variational equations

With $I = I(x_1, \dots, x_{2n+3}, t) =$ const. the invariant (1.29) of the Hamiltonian system (1.17), we may straightforwardly prove that the quantity J, given by [20]

$$J = \delta I = \sum_{i=1}^{2n+3} \frac{\partial I}{\partial x_i}\,\delta x_i \tag{1.55}$$

is a constant of motion pertaining to the extended systems of $4n+6$ first order equations (1.53) and (1.54). The invariant J thus provides a relation between the instantaneous shape of the phase-space surface defined by the invariant I and the infinitesimal deviation $\delta\vec{x}$ that represents a neighboring system.

The prove is worked out directly by showing that $dJ/dt = 0$, which means explicitly

$$\begin{aligned}
\frac{d}{dt}J &= \sum_{i=1}^{2n+3} \frac{d}{dt}\left(\frac{\partial I}{\partial x_i}\delta x_i\right) \\
&= \sum_{i=1}^{2n+3}\left[\delta x_i \frac{\partial}{\partial t}\left(\frac{\partial I}{\partial x_i}\right) + \delta x_i \sum_{j=1}^{2n+3} \dot{x}_j \frac{\partial}{\partial x_j}\left(\frac{\partial I}{\partial x_i}\right) + \frac{\partial I}{\partial x_i}\frac{d}{dt}\delta x_i\right] \\
&= \sum_{i=1}^{2n+3}\left[\delta x_i \frac{\partial}{\partial t}\left(\frac{\partial I}{\partial x_i}\right) + \delta x_i \sum_{j=1}^{2n+3} f_j \frac{\partial}{\partial x_j}\left(\frac{\partial I}{\partial x_i}\right) + \sum_{j=1}^{2n+3} \delta x_j \frac{\partial I}{\partial x_i}\frac{\partial f_i}{\partial x_j}\right] .
\end{aligned}$$

Interchanging the order of summation, and subsequently renaming the summation indices, the last sum takes on the equivalent forms

$$\sum_{i=1}^{2n+3}\sum_{j=1}^{2n+3} \delta x_j \frac{\partial I}{\partial x_i}\frac{\partial f_i}{\partial x_j} = \sum_{i=1}^{2n+3}\sum_{j=1}^{2n+3} \delta x_i \frac{\partial I}{\partial x_j}\frac{\partial f_j}{\partial x_i} .$$

The total time derivative of J thus takes the form

$$\begin{aligned}
\frac{d}{dt}J &= \sum_{i=1}^{2n+3} \delta x_i \left[\frac{\partial}{\partial x_i}\left(\frac{\partial I}{\partial t}\right) + \sum_{j=1}^{2n+3}\left\{ f_j \frac{\partial}{\partial x_i}\left(\frac{\partial I}{\partial x_j}\right) + \frac{\partial I}{\partial x_j}\frac{\partial f_j}{\partial x_i}\right\}\right] \\
&= \sum_{i=1}^{2n+3} \delta x_i \frac{\partial}{\partial x_i}\left[\frac{\partial I}{\partial t} + \sum_{j=1}^{2n+3} f_j \frac{\partial I}{\partial x_j}\right] \\
&= \sum_{i=1}^{2n+3} \delta x_i \frac{\partial}{\partial x_i}\left(\frac{dI}{dt}\right) \\
&= 0 ,
\end{aligned}$$

since $dI/dt = 0$ for the system's constant of motion I. The stability analysis of the extended system provides both the stability of the non-extended system and the stability of the phase-space symmetry surface, as described by the invariant I.

1.3 Physical interpretation of the invariant I

The invariant (1.29) is easily shown to represent a time integral of the auxiliary equation (1.27) by calculating the total time derivative of (1.29), and inserting the canonical equations (1.18). Hence, Eq. (1.29) provides a conserved quantity exactly along the phase-space trajectory that represents the system's time evolution. This trajectory is given as a solution of the $2n$ first-order canonical equations (1.18) or, equivalently, of the n second-order equations of motion (1.18a). With these solutions, Eq. (1.27) must not be conceived as a conditional equation for the potential $V(\vec{q}, t)$. Rather, all q_i-dependent terms of Eq. (1.27) are in fact functions of the parameter t only — given along the system's phase-space trajectory. Correspondingly, the potential $V(\vec{q}(t), t)$ and its derivatives in (1.27) are time-dependent coefficients of an ordinary third-order differential equation for $\xi(t)$. Thus, the $2n$ first-order canonical equations that uniquely determine the time evolution of the n particle system form together with the three first-order equations of the auxiliary equation for $\xi(t)$ a closed coupled set of $2n+3$ first-order equations that uniquely determine $\xi(t)$. According to the existence and uniqueness theorem for linear ordinary differential equations, a unique solution function $\xi(t)$ of Eq. (1.27) exists — and consequently the invariant I — if V and its partial derivatives are continuous along the system's phase-space path.

Vice versa, Eq. (1.27) together with the side-condition $I = \text{const.}$ from Eq. (1.29) may be conceived as a conditional equation for a potential $V(\vec{q},t)$ that is consistent with a solution of the equations of motion (1.18). In other words, the invariant $I = \text{const.}$ in conjunction with the third-order equation (1.27) must imply the canonical equations (1.18). This can be shown inserting Eq. (1.27) into the total time derivative of (1.29). Since $dI/dt \equiv 0$ must hold for all solutions $\xi(t)$ of Eq. (1.27), the respective sums of terms proportional to $\ddot{\xi}(t)$, $\dot{\xi}(t)$, and $\xi(t)$ must vanish separately. For the terms proportional to $\ddot{\xi}(t)$, this means

$$\tfrac{1}{2}\ddot{\xi}\, e^{F(t)} \sum_{i=1}^{n} q_i \left(\dot{q}_i - p_i\, e^{-F}\right) \equiv 0\,. \tag{1.56}$$

The identity (1.56) must be fulfilled for *all* initial conditions $(\vec{q}(0), \vec{p}(0))$ and resulting phase-space trajectories $(\vec{q}(t), \vec{p}(t))$ of the underlying dynamical system. Consequently, the expression in parentheses must vanish separately for each index i, thereby establishing the first canonical equation (1.18). The remaining terms impose the following condition for a vanishing total time derivative of I

$$e^{-F(t)} \sum_{i=1}^{n} \left(\xi\, p_i - \tfrac{1}{2}\, e^{F} \left(\dot{\xi} - \xi f\right) q_i\right) \left(\dot{p}_i + \frac{\partial V}{\partial q_i} e^{F}\right) \equiv 0\,.$$

Again, this sum must vanish for all $\xi(t)$ that are solution of Eq. (1.27). This can be accomplished only if the rightmost expression in parentheses, hence the second canonical equation (1.18), is fulfilled for each index $i = 1, \ldots, n$. Summarizing, we may state that the triple made up by the canonical equations (1.18), the auxiliary equation (1.27), and the invariant I of Eq. (1.29) forms a logical triangle: if two equations are given at a time, the third can be deduced.

The physical interpretation of the invariant (1.29) can be worked out considering the total time derivative of the Hamiltonian (1.17). Making use of the canonical equations (1.18), we find

$$\frac{dH}{dt} + \tfrac{1}{2} f e^{-F} \sum_{i=1}^{n} p_i^2 - e^{F} \left(f V(\vec{q},t) + \frac{\partial V}{\partial t}\right) = 0\,, \tag{1.57}$$

which represents just the explicit form of the general theorem $dH/dt = \partial H/\partial t$ for the Hamiltonian (1.17). Equation (1.57) can be interpreted as an energy balance relation, stating that the system's total energy change dH/dt is quantified by the dissipation and the explicit time-dependence of the external potential. Inserting $\partial V/\partial t$ from the auxiliary equation (1.27) into Eq. (1.57), the sum over all terms can be written as the total time derivative

$$\frac{d}{dt}\left[\xi H - \tfrac{1}{2}\left(\dot{\xi} - \xi f\right) \sum_{i=1}^{n} q_i\, p_i + \tfrac{1}{4} e^{F} \left(\ddot{\xi} - \dot{\xi} f - \xi \dot{f}\right) \sum_{i=1}^{n} q_i^2\right] = 0\,.$$

The expression in brackets coincides with the invariant (1.29). As the function $\xi(t)$ is the solution of a homogeneous linear differential equation (1.27), it is determined up to an arbitrary factor. We are, therefore, free to conceive $\xi(t)$ as a dimensionless quantity.

With the initial conditions $\xi(0) = 1$, $\dot{\xi}(0) = \ddot{\xi}(0) = 0$ for the auxiliary equation (1.27), the invariant I can now be interpreted as the conserved *initial* energy H_0 for a non-autonomous system described by the Hamiltonian (1.17), comprising both the system's time-varying energy content H and the energy fed into or detracted from the system.

The meaning of $\xi(t)$ follows directly from the invariant $I = I(\vec{q}, \vec{p}, t, \mathcal{H})$ of Eq. (1.29) treating the Hamiltonian $H = \mathcal{H}$ formally as an independent variable. A vanishing total differential of the invariant I then writes

$$dI \equiv \left.\frac{\partial I}{\partial t}\right|_{\vec{q},\vec{p},\mathcal{H}} dt + \left.\frac{\partial I}{\partial \mathcal{H}}\right|_{\vec{q},\vec{p},t} d\mathcal{H} + \sum_{i=1}^{n} \left(\left.\frac{\partial I}{\partial q_i}\right|_{\vec{p},t,\mathcal{H}} dq_i + \left.\frac{\partial I}{\partial p_i}\right|_{\vec{q},t,\mathcal{H}} dp_i \right) = 0\,.$$

Inserting q_i and p_i from the canonical equations (1.18), and making again use of the auxiliary equation (1.27) to eliminate the third-order derivative $\dddot{\xi}(t)$ that is contained in the explicit expression for $\partial I/\partial t$, we find the expected result

$$\frac{\partial I}{\partial \mathcal{H}}\bigg|_{\vec{q},\vec{p},t} = \xi(t)\,. \tag{1.58}$$

$\xi(t)$ thus quantifies the change ΔI of the total energy content of a "neighboring" system with an invariant $I + \Delta I$ with respect to a change of the actual system energy $\mathcal{H} = H$ at fixed phase-space location $(\vec{q}, \vec{p})$ and time t.

For the special case $f(t) \equiv \partial V/\partial t \equiv 0$, hence for autonomous systems, $\xi(t) \equiv 1$ is always a solution of Eq. (1.27). For this $\xi(t)$, the invariant (1.29) reduces to $I \equiv H$, hence provides the system's total energy, which is a known invariant for Hamiltonian systems with no explicit time-dependence. Nevertheless, Eq. (1.27) also admits solutions $\xi(t) \neq$ const. for these systems. We thereby obtain other non-trivial invariants for autonomous systems that exist in addition to the invariant representing the energy conservation law. This will be demonstrated for the simple case of the harmonic oscillator at the end of Sec. 1.4.1.

For general potentials $V(\vec{q}, t)$, the dependence of Eq. (1.27) on $\vec{q}(t)$ cannot be eliminated. Under these circumstances, the function $\xi(t)$ can only be obtained integrating (1.27) *simultaneously* with the equations of motion (1.18a). For the isotropic quadratic potential with $d(t)$ denoting an arbitrary continuous function of time

$$V(\vec{q}, t) = d(t) \sum_{i=1}^{n} q_i^2\,, \tag{1.59}$$

Equation (1.27) may be divided by $\sum_i q_i^2$ and hereby strip its dependence on the single particle trajectories $q_i(t)$. Only for the particular linear system associated with (1.59), the third-order differential equation (1.27) for $\xi(t)$ decouples from the equations of motion (1.18a). Then, the solution functions $\xi(t)$, $\dot{\xi}(t)$, and $\ddot{\xi}(t)$ apply to all trajectories that follow from the equations of motion (1.18a) with (1.59). For the potential (1.59), Eq. (1.27) may be integrated to yield a non-linear second-order equation for $\xi(t)$

$$\ddot{\xi}\xi - \tfrac{1}{2}\dot{\xi}^2 + \xi^2\Big[4d - \dot{f} - \tfrac{1}{2}f^2\Big] = c\,, \tag{1.60}$$

$c =$ const. denoting the integration constant. With the help of Eq. (1.60), we may eliminate $\ddot{\xi}(t)$ in the expression (1.29) for the invariant I. After reordering, Eq. (1.29) may then be rewritten as

$$8\xi\, I = e^{F(t)} \sum_{i=1}^{n} \left(\Big[2\xi \dot{q}_i - \big(\dot{\xi} - \xi f\big) q_i\Big]^2 + 2c\, q_i^2 \right)\,. \tag{1.61}$$

Obviously, for a positive integration constant $c > 0$, the quantities I and $\xi(t)$ must have the same sign. Thus, for $c > 0$, an invariant $I > 0$, and for the initial condition $\xi(0) > 0$, the function $\xi(t)$ remains non-negative at all times $t > 0$ for systems governed by the potential (1.59). On the other hand, $\xi(t)$ may change sign for general non-linear systems (1.17). As has been shown in Sec. 1.2.1, the condition $\xi(t) > 0$ provides a necessary criterion for the *physical* existence of an equivalent autonomous system of (1.17).

1.4 Examples of time-dependent Hamiltonian systems

1.4.1 Time-dependent damped harmonic oscillator

As a simple example, we treat the well-known one-dimensional time-dependent harmonic oscillator with damping forces linear in the velocity. Its Hamiltonian is given by

$$H = \tfrac{1}{2}p^2 e^{-F(t)} + \tfrac{1}{2}\omega^2(t)\, q^2 e^{F(t)}\,, \tag{1.62}$$

which yields the equation of motion

$$\dot{q} = p\, e^{-F(t)}\,, \qquad \ddot{q} + f(t)\,\dot{q} + \omega^2(t)\, q = 0\,. \tag{1.63}$$

Because of the quadratic structure of the potential $V(q,t) = \frac{1}{2}\omega^2(t)\, q^2$, the dependence of the auxiliary equation (1.27) on the particle coordinate q cancels. The differential equation for $\xi(t)$ thus simplifies to

$$\dddot{\xi} + \dot{\xi}\left(4\omega^2 - 2\dot{f} - f^2\right) + \xi\left(4\omega\dot{\omega} - \ddot{f} - f\dot{f}\right) = 0\,. \tag{1.64}$$

The invariant I is immediately found as the one-degree-of-freedom version of Eq. (1.29)

$$I = \xi\, H - \tfrac{1}{2}\Big(\dot{\xi} - \xi\, f\Big) q\, p + \tfrac{1}{4}e^{F(t)}\left(\ddot{\xi} - \dot{\xi}f - \xi\dot{f}\right) q^2\,, \tag{1.65}$$

with H standing for the Hamiltonian (1.62). For this particular case, the linear third-order equation (1.64) for $\xi(t)$ can be integrated once to yield a non-linear second-order equation

$$\xi\ddot{\xi} - \tfrac{1}{2}\dot{\xi}^2 + 2\xi^2\left(\omega^2 - \tfrac{1}{2}\dot{f} - \tfrac{1}{4}f^2\right) = 2c\,, \tag{1.66}$$

$c =$ const. denoting the integration constant. Using Eq. (1.66) to replace $\ddot{\xi}(t)$ in Eq. (1.65), we obtain the invariant I for the system (1.62) in the alternative form

$$I = \frac{ce^F}{2\xi}q^2 + \tfrac{1}{2}\left(p\sqrt{\xi/e^F} - \tfrac{1}{2}q\left[\dot{\xi} - \xi f\right]\sqrt{e^F/\xi}\right)^2. \tag{1.65a}$$

As already concluded from Eq. (1.61), $\xi(t)$ cannot change sign if we define $c > 0$. The substitution $\xi(t) = \rho^2(t)$ then exists for real $\rho(t)$ at all times t, which means that Eqs. (1.66) and (1.65a) can be expressed equivalently in terms of $\rho(t)$. Setting $c = 1$, this leads to the auxiliary equation and the invariant in the form derived by Leach [14], who applied the method of linear canonical transformations with time-dependent coefficients.

The expression for the invariant (1.65) becomes particularly simple if expressed in terms of the coordinates of the canonically transformed system. Applying the related transformation rules (1.22), we find, inserting Eq. (1.66)

$$I = \tfrac{1}{2}p'^2 + \tfrac{1}{2}c\, q'^2\,. \tag{1.67}$$

According to the canonical transformation theory of Sec. 1.2.1, the invariant I may regarded as the Hamiltonian H' of an autonomous system that is equivalent to (1.62)

$$H' = \tfrac{1}{2}p'^2 + V'(q')\,, \tag{1.68}$$

with the effective potential (1.25) in the transformed system simplifying to

$$V'(q') = \tfrac{1}{4}\Big[\ddot{\xi}\xi - \tfrac{1}{2}\dot{\xi}^2 + 2\xi^2\big(\omega^2 - \tfrac{1}{2}\dot{f} - \tfrac{1}{4}f^2\big)\Big]q'^2\,.$$

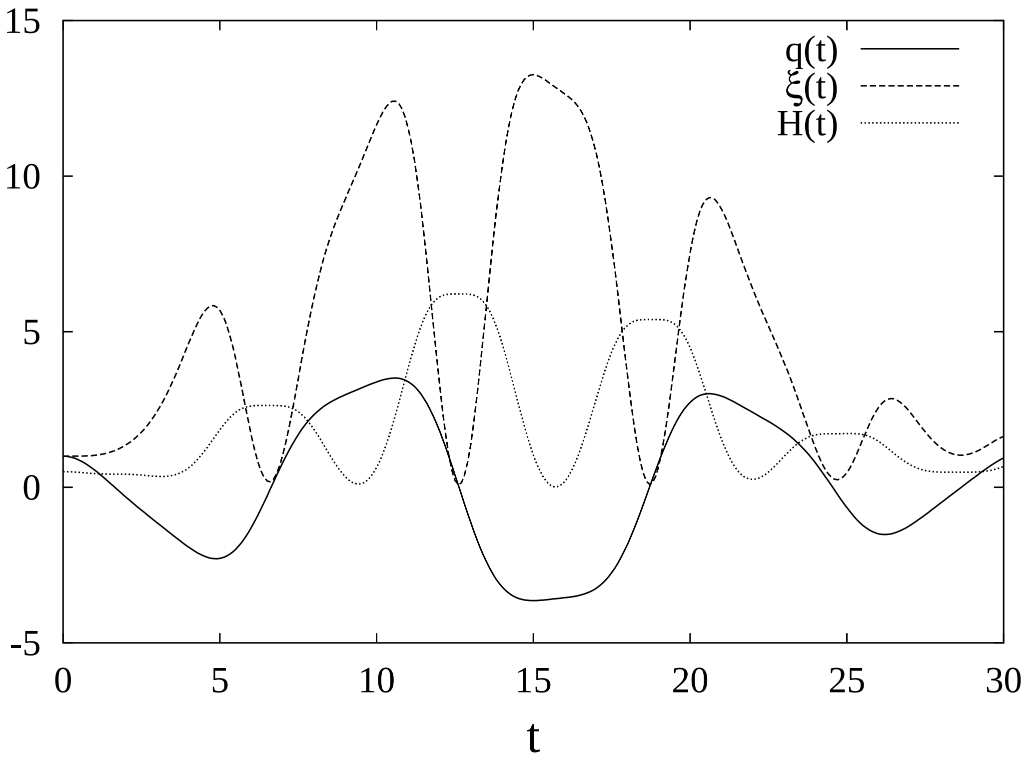

Figure 1.1: Example of a simultaneous numerical integration of the equation of motion (1.63) and the auxiliary equation (1.64). In addition, $H(t)$ displays the actual system energy given by the Hamiltonian (1.62).

Comparing the expression in brackets with (1.66), we find that the new Hamiltonian (1.68) indeed agrees with the invariant (1.67). Fig. 1.1 shows a special case of a numerical integration of the equation of motion (1.63). The results of the simultaneous numerical integration of the auxiliary equation Eqs. (1.64) are included in this figure. As coefficients of Eq. (1.63) we chose

$$\omega(t) = \cos(t/2)\,, \quad f(t) = 1.8 \times 10^{-2} \sin(t/\pi)\,.$$

The initial conditions were set to $q(0) = 1$, $\dot{q}(0) = 0$, $\xi(0) = 1$, $\dot{\xi}(0) = 0$, and $\ddot{\xi}(0) = 0$. According to (1.65), we hereby define an invariant of $I = H(0) = 0.5$ for the sample particle.

In agreement with Eq. (1.61), the function $\xi(t)$ remains positive for this linear system. We furthermore observe that $\xi(t)$ is related to the energy transfer into the system according to Eq. (1.58): $\xi(t)$ becomes large for strong changes of the actual system energy $H(t)$ — and vice versa.

For the time-independent version of Eq. (1.62), we have $\dot{\omega}, f, \dot{f} \equiv 0$, hence $\omega \equiv \omega_0$. The auxiliary equation (1.64) then further simplifies to

$$\dddot{\xi} + 4\omega_0^2\,\dot{\xi} = 0\,. \tag{1.69}$$

With the integration constants a_0, a_1, and a_2, Eq. (1.69) has the general solution

$$\xi(t) = a_0 + a_1 \cos 2\omega_0 t + a_2 \sin 2\omega_0 t\,.$$

The solution of the equation of motion (1.63) for this system contains two constants, $q_0 = q(0)$ and $p_0 = p(0)$

$$q(t) = q_0 \cos\omega_0 t + p_0\omega_0^{-1} \sin\omega_0 t\,, \qquad p(t) = -q_0\omega_0 \sin\omega_0 t + p_0 \cos\omega_0 t\,.$$

The particular invariants for the time-independent harmonic oscillator now follow from

$$I = \tfrac{1}{2}\xi(t)\left(p^2 + \omega_0^2 q^2\right) - \tfrac{1}{2}\dot{\xi}(t)\, pq + \tfrac{1}{4}\ddot{\xi}(t)\, q^2\,. \tag{1.70}$$

For the special solution $\xi(t) \equiv 1$ of Eq. (1.69), hence for $a_0 = 1$, $a_1 = a_2 = 0$, the invariant coincides with the system's Hamiltonian $I \equiv H$, which represents the conserved total energy of this autonomous system. Setting $a_1 = 1$ and $a_0 = a_2 = 0$, the solution of the auxiliary equation (1.69) reads $\xi(t) = \cos 2\omega_0 t$. Then, Eq. (1.70) leads to the second non-trivial invariant of the harmonic oscillator, as derived by Lutzky [21]

$$I = \tfrac{1}{2}\left(p^2 - \omega_0^2 q^2\right)\cos 2\omega_0 t + qp\,\omega_0 \sin 2\omega_0 t\,.$$

The five integration constants correspond to the five-parameter Noether subgroup of the complete eight-parameter symmetry group $\mathrm{SL}(3,\mathbb{R})$ for the harmonic oscillator [22].

1.4.2 Time-dependent anharmonic undamped oscillator

As a second example, we investigate the one-dimensional non-linear system of a time-dependent anharmonic oscillator without damping, defined by the Hamiltonian

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2(t)\, q^2 + a(t)\, q^3 + b(t)\, q^4\,. \tag{1.71}$$

The associated equation of motion is given by

$$\dot{q} = p\,, \qquad \ddot{q} + \omega^2(t)\, q + 3a(t)\, q^2 + 4b(t)\, q^3 = 0\,. \tag{1.72}$$

Again, the invariant is immediately obtained writing the general invariant (1.29) for one dimension. With vanishing damping functions ($F(t), f(t) \equiv 0$), the invariant simplifies to

$$I = \tfrac{1}{2}\xi(t)\left[\dot{q}^2 + \omega^2(t)\, q^2 + 2a(t)\, q^3 + 2b(t)\, q^4\right] - \tfrac{1}{2}\dot{\xi}(t)\, q\dot{q} + \tfrac{1}{4}\ddot{\xi}(t)\, q^2\,. \tag{1.73}$$

For this particular case, the linear third-order equation for the auxiliary function $\xi(t)$ reads

$$\dddot{\xi} + 4\dot{\xi}\,\omega^2(t) + 4\xi\,\omega\,\dot{\omega} + 2q(t)\left[2\xi\,\dot{a} + 5\dot{\xi}\,a\right] + 4q^2(t)\left[\xi\,\dot{b} + 3\dot{\xi}\,b\right] = 0\,, \tag{1.74}$$

which follows from the general form of Eq. (1.27). We observe that — in contrast to the previous linear example — the particle trajectory $q = q(t)$ is explicitly contained in in the related auxiliary equation (1.74). Consequently, the integral function $\xi(t)$ can only be determined if (1.74) is integrated *simultaneously* with the equation of motion (1.72).

We may directly convince ourselves that I is indeed a conserved quantity. Calculating the total time derivative of Eq. (1.73), and inserting the equation of motion (1.72), we end up with Eq. (1.74), which is fulfilled by definition of $\xi(t)$ for the given trajectory $q = q(t)$. The third-order differential equation (1.74) may be converted into a coupled set of first- and second-order equations. It is easily shown that the non-linear second-order equation

$$\xi\ddot{\xi} - \tfrac{1}{2}\dot{\xi}^2 + 2\omega^2(t)\,\xi^2 = g(t) \tag{1.75}$$

is equivalent to (1.74), provided that the time derivative of the function $g(t)$, introduced in (1.75), is given by

$$\dot{g}(t) = -2q(t)\,\xi\left[2\xi\,\dot{a} + 5\dot{\xi}\,a\right] - 4q^2(t)\,\xi\left[\xi\,\dot{b} + 3\dot{\xi}\,b\right]. \tag{1.76}$$

With the help of the auxiliary equation in the form of Eq. (1.75), the invariant (1.73) may be expressed equivalently as

$$I = \tfrac{1}{2}\left[\xi\,\dot{q}^2 - \dot{\xi}\,q\dot{q} + \frac{\dot{\xi}^2}{4\xi}\,q^2 + 2\xi\,a\,q^3 + 2\xi\,b\,q^4\right] + \frac{g(t)}{4\xi}\,q^2\,. \tag{1.77}$$

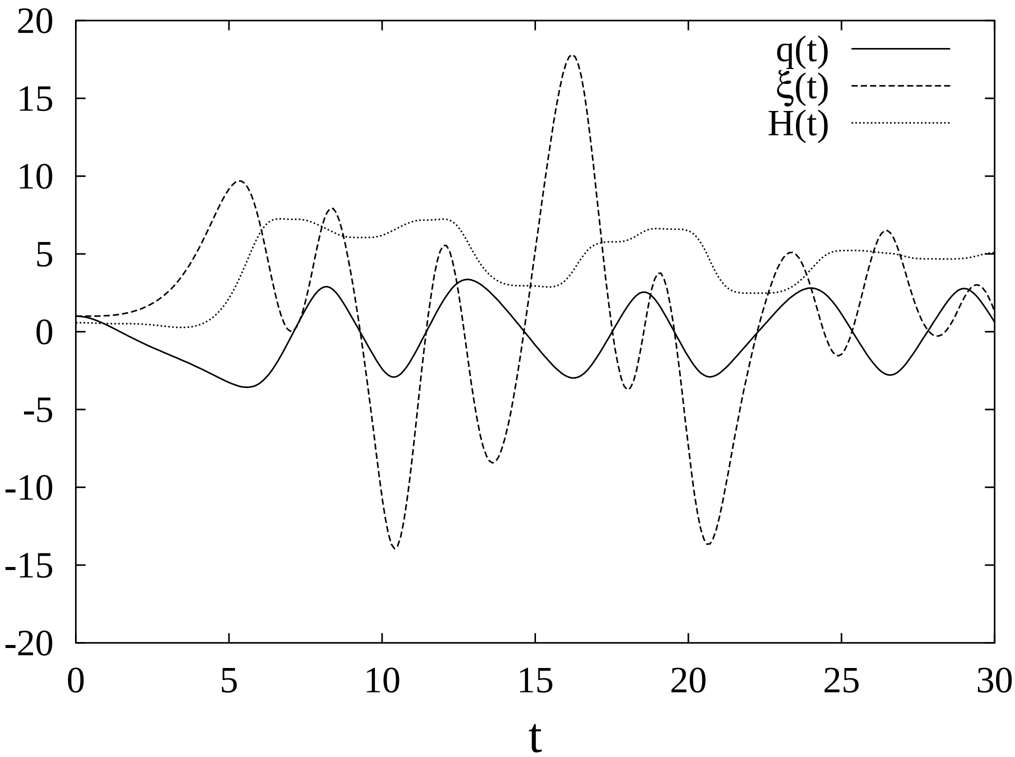

Figure 1.2: Example of a simultaneous numerical integration of the equation of motion (1.72) and the coupled set (1.75), (1.76) for $\xi(t)$. In addition, $H(t)$ displays the time-dependent system energy given by the Hamiltonian (1.71).

In contrast to Eq. (1.74), the equivalent coupled set of equations (1.75) and (1.76) does not contain anymore the time derivative of the external function $\omega^2(t)$.

For the time-dependent harmonic oscillator $(a(t) = \dot{a}(t) = b(t) = \dot{b}(t) \equiv 0)$, Eq. (1.76) leads to $\dot{g}(t) = 0$, which means that $g(t) = g_0 =$ const. For this particular case, g_0, and hence Eq. (1.75) no longer depends on the specific particle trajectory $q = q(t)$. Consequently, the solution function $\xi(t)$ applies to arbitrary trajectories. Setting $g_0 = 2$ and $\xi(t) = \rho^2(t)$ we obtain the well-known Lewis invariant [14]

$$I = \tfrac{1}{2}\left[\rho^{-2}q^2 + (\rho\dot{q} - \dot{\rho}q)^2\right] .$$

For this linear case, we can rewrite Eq. (1.77) as

$$8I\xi(t) = \left[2\xi(t)\dot{q} - q\dot{\xi}(t)\right]^2 + 2q^2 g_0 ,$$

providing a special case of the general Eq. (1.61). For the initial condition $g_0 > 0$, and $I > 0$, we have $\xi(t) \geq 0$ for all $t > 0$. As a consequence, the linear canonical transformation (1.22) is regular for all times t, and the equivalent autonomous system represents a real physical system. In contrast, the function $g(t)$ is no longer a constant in the general non-linear case, and $\xi(t)$ may become negative. For $\xi(t) < 0$, the canonical transformation (1.22) becomes imaginary, which means that the equivalent system is no longer physical. Nevertheless, the invariant (1.73) exists as a real number for all solutions of the third-order differential equation (1.74), independently of the sign of $\xi(t)$.

Fig. 1.2 shows a special case of a numerical integration of the equation of motion (1.72). Included in this figure, we see the result of the simultaneous numerical integration of Eqs. (1.75) and (1.76). The coefficients of Eq. (1.72) were chosen as

$$\omega(t) = \cos(t/2) , \quad a(t) = 5 \times 10^{-2} \sin(t/3) , \quad b(t) = 8 \times 10^{-2} \cos^2(t/3) .$$

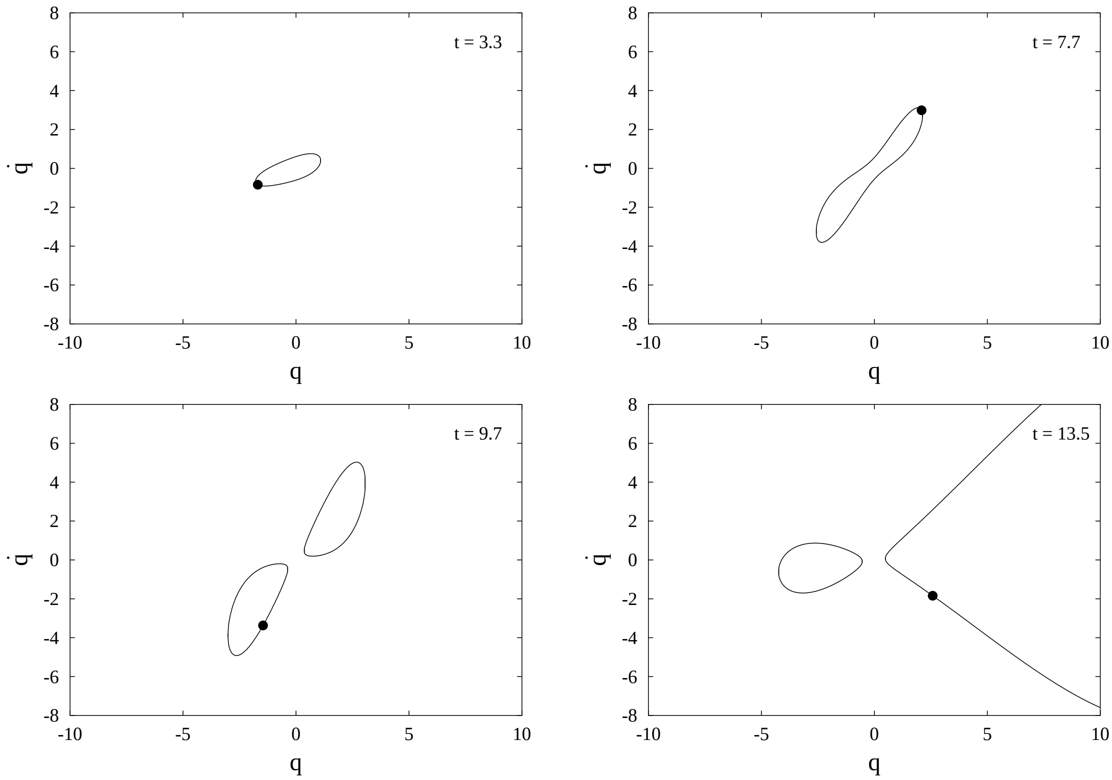

Figure 1.3: Lines of constant invariant $I = 0.58$ in the $(q, \dot{q})$ phase-space plane and location of the sample particles at the instants of time $\xi(t = 3.3) = 3.2$, $\xi(t = 7.7) = 3.7$, $\xi(t = 9.7) = -6.1$, and $\xi(t = 13.5) = -8.3$.

The initial conditions were set to $q(0) = 1$, $\dot{q}(0) = 0$, $\xi(0) = 1$, $\dot{\xi}(0) = 0$, and $\ddot{\xi}(0) = 0$. According to (1.77), we hereby define an invariant of $I = H(0) = 0.58$ for the sample particle. Owing to the system's non-linear dynamics, $\xi(t)$ now becomes piecewise negative. Also, the relationship (1.58) between $\xi(t)$ and $H(t)$ appears more complicated compared to the linear case of Fig. 1.1. Interesting insight into the dynamical evolution of the sample particle can be obtained if the invariant (1.77) is regarded as an implicit representation of a phase-space curve $I = I(q, \dot{q}, t)$. Fig. 1.3 displays snapshots of these curves at four different instants of time t. As expected, the particle lies exactly on these curves of constant I, thereby providing a numerical verification of Eq. (1.77). The two upper pictures display situations with $\xi(t) > 0$. Then, the phase-space curves are of closed elliptic type, being more or less deformed because of the non-linear terms in the Hamiltonian (1.71). When the function $\xi(t)$ becomes negative, as given for the lower two pictures, topological changes of the phase-space curves to more complex shapes are observed. For the special case of a conservative system, we have $\omega(t) = \omega_0 = \text{const.}$, $a(t) = a_0 = \text{const.}$, $b(t) = b_0 = \text{const.}$, and Eq. (1.74) reduces to

$$\dddot{\xi}(t) + \dot{\xi}(t)\big[4\omega_0^2 + 10q(t)a_0 + 12q^2(t)\,b_0\big] = 0\,. \tag{1.78}$$

Obviously, this equation has the special solution $\xi(t) \equiv 1$. For this case, Eq. (1.73) simplifies to

$$I = \tfrac{1}{2}\dot{q}^2 + \tfrac{1}{2}\omega_0^2 q^2 + a_0 q^3 + b_0 q^4 = H\,,$$

thus agrees with the system's Hamiltonian, which represents the conserved total energy. Another non-trivial invariant is obtained inserting a solution of the auxiliary equation (1.78) with $\xi(t) \neq \text{const.}$ into the expression for the invariant (1.73).

1.4.3 Invariant for a system of Coulomb-interacting particles in external potentials

We now analyze a three-dimensional example, namely, an ensemble of N Coulomb-interacting particles of the same species moving in a time-dependent quadratic external potential, as typically given in the co-moving frame for charged particle beams that propagate through linear focusing lattices. The particle coordinates in the three spatial directions are distinguished by x_i, y_i, and z_i, the canonical momenta correspondingly by $p_{x,i}$, $p_{y,i}$, and $p_{z,i}$. With a vanishing friction $f(t) \equiv 0$, the Hamiltonian H of this system may be written as

$$H = \sum_{i=1}^{N} \tfrac{1}{2}\big(p_{x,i}^2 + p_{y,i}^2 + p_{z,i}^2\big) + V\big(\vec{x}, \vec{y}, \vec{z}, t\big)\,. \tag{1.79}$$

The effective potential contained herein is given by

$$V\big(\vec{x}, \vec{y}, \vec{z}, t\big) = \sum_{i=1}^{N} \Big[\tfrac{1}{2}\omega_x^2(t)\, x_i^2 + \tfrac{1}{2}\omega_y^2(t)\, y_i^2 + \tfrac{1}{2}\omega_z^2(t)\, z_i^2 + \tfrac{1}{2}\sum_{j\neq i}\frac{c_1}{r_{ij}}\Big]\,, \tag{1.80}$$

with $r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$ and $c_1 = q^2/4\pi\epsilon_0 m$, q and m denoting the particles' charge and mass, respectively. The equations of motion that follow from (1.79) with (1.80) are

$$\dot{x}_i = p_{x,i}\,, \quad \ddot{x}_i + \omega_x^2(t)\, x_i - c_1 \sum_{j\neq i} \frac{x_i - x_j}{r_{ij}^3} = 0\,, \tag{1.81}$$

and likewise for the y- and z-directions. We note that the factor $1/2$ in front of the Coulomb interaction term in (1.80) disappears in Eq. (1.81) since each term occurs twice in the symmetric form of the double sum.

For the effective potential (1.80) and $f(t) \equiv 0$, the third-order differential equation (1.27) for ξ specializes to

$$\begin{aligned}\sum_i \Big[x_i^2 \Big(\dddot{\xi} + 4\dot{\xi}\omega_x^2 + 4\xi\omega_x\dot{\omega}_x\Big) + y_i^2 \Big(\dddot{\xi} + 4\dot{\xi}\omega_y^2 + 4\xi\omega_y\dot{\omega}_y\Big) \\ + z_i^2 \Big(\dddot{\xi} + 4\dot{\xi}\omega_z^2 + 4\xi\omega_z\dot{\omega}_z\Big) + \dot{\xi}\sum_{j\neq i}\frac{c_1}{r_{ij}}\Big] = 0\,.\end{aligned} \tag{1.82}$$

With $\xi(t)$ a solution of (1.82) and H the Hamiltonian (1.79), the invariant follows directly from (1.29) as

$$I = \xi(t)\, H - \tfrac{1}{2}\dot{\xi}\sum_i \big(x_i\, p_{x,i} + y_i\, p_{y,i} + z_i\, p_{z,i}\big) + \tfrac{1}{4}\ddot{\xi}\sum_i \big(x_i^2 + y_i^2 + z_i^2\big)\,. \tag{1.83}$$

Equation (1.82) may be cast into a compact form if the sums over the particle coordinates are written in terms of "second beam moments", denoted as $\langle x^2 \rangle$ for the x coordinates. Likewise, the double sum over the Coulomb interaction terms may be expressed as the electric field energy $W(t)$ of all particles

$$\langle x^2 \rangle(t) = \frac{1}{N}\sum_i x_i^2(t)\,, \quad W(t) = \frac{m}{2}\sum_i\sum_{j\neq i}\frac{c_1}{r_{ij}}\,.$$

The similar notation will be used for all quadratic terms of the particle coordinates. Corresponding to the previous example, the third-order equation (1.82) may be split into a coupled set of first- and second-order differential equations. Similar to Eq. (1.66), we write the non-linear second-order equation for $\xi(t)$ as

$$\xi\ddot{\xi} - \tfrac{1}{2}\dot{\xi}^2 + 2\xi^2\,\omega^2(t) = 2g(t)\,. \tag{1.84}$$

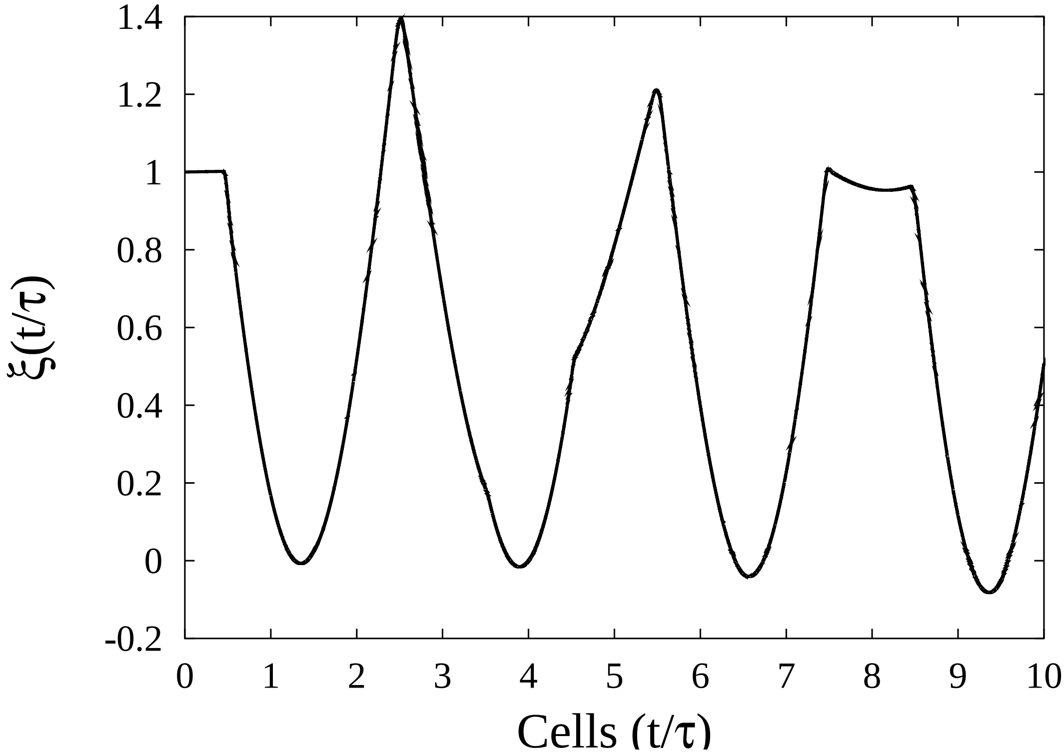

Figure 1.4: $\xi(t)$ as stable solution of (1.82) for $\sigma_0 = 45°$, $\sigma = 9°$. τ denotes the focusing period common to all three directions.

The function $\omega^2(t)$ contained herein is defined as the "average focusing function" according to

$$\omega^2(t) = \frac{\omega_x^2 \left\langle x^2 \right\rangle + \omega_y^2 \left\langle y^2 \right\rangle + \omega_z^2 \left\langle z^2 \right\rangle}{\left\langle x^2 \right\rangle + \left\langle y^2 \right\rangle + \left\langle z^2 \right\rangle} \,.$$

Comparing the time derivative of Eq. (1.84) with (1.82), one finds that the time derivative of $g(t)$ must satisfy

$$\dot{g}(t) = \frac{1}{\left\langle x^2 \right\rangle + \left\langle y^2 \right\rangle + \left\langle z^2 \right\rangle} \Bigg[2\xi^2 \Big\{ \left\langle x p_x \right\rangle \left(\omega_x^2 - \omega^2\right) + \left\langle y p_y \right\rangle \left(\omega_y^2 - \omega^2\right) + \left\langle z p_z \right\rangle \left(\omega_z^2 - \omega^2\right) \Big\} - \xi\dot{\xi} \frac{W}{mN} \Bigg] \,. \tag{1.85}$$

Unlike the third-order equation (1.82), the equivalent coupled set of equations (1.84) and (1.85) no longer contains the time derivatives of the external focusing functions $\omega_x(t)$, $\omega_y(t)$, and $\omega_z(t)$. We observe that $\dot{g}(t)$ is determined by two quantities of different physical nature: the field energy constituted by all particles as a measure for the strength of the Coulomb interaction, and the system's anisotropy. In contrast to the right hand side of Eq. (1.66) pertaining to the one-dimensional example of Sec. 1.4.1, the function $g(t)$ is generally *not* constant if the system is not strictly isotropic — even in the linear case, which is given here for a vanishing Coulomb interaction ($W \to 0$).

With the help of (1.84), we may substitute $\ddot{\xi}(t)$ and the external focusing functions in (1.83) to express the invariant in the alternative form

$$2\xi I/N = \left\langle \left(\xi p_x - \tfrac{1}{2}\dot{\xi} x\right)^2 \right\rangle + \left\langle \left(\xi p_y - \tfrac{1}{2}\dot{\xi} y\right)^2 \right\rangle + \left\langle \left(\xi p_z - \tfrac{1}{2}\dot{\xi} z\right)^2 \right\rangle + \xi^2(t) \frac{2W}{mN} + g(t) \left(\left\langle x^2 \right\rangle + \left\langle y^2 \right\rangle + \left\langle z^2 \right\rangle \right) \,. \tag{1.86}$$

Similar to the previous example, the function $g(t)$ accounts for an eventual change of sign of $\xi(t)$, owing to the fact that all other terms on the right hand side of Eq. (1.86) may not turn negative.

The canonical transformation (1.22) becomes undefined for instants of time t with $\xi(t) = 0$. Furthermore, for time intervals with a negative value of $\xi(t)$, the elements of the transformation matrix (1.22) turn imaginary. For these cases, the equivalent autonomous system of (1.79), (1.80) that is defined by the canonical transformation generated by (1.20) ceases to exist in a physical sense. This indicates that the beam evolves within the non-autonomous system in a way that can no longer be correlated to the beam evolution within an autonomous system by the linear canonical transformation (1.22). In contrast, the invariant (1.83) itself exists for *all* $\xi(t)$ that are solutions of the auxiliary equation (1.82).

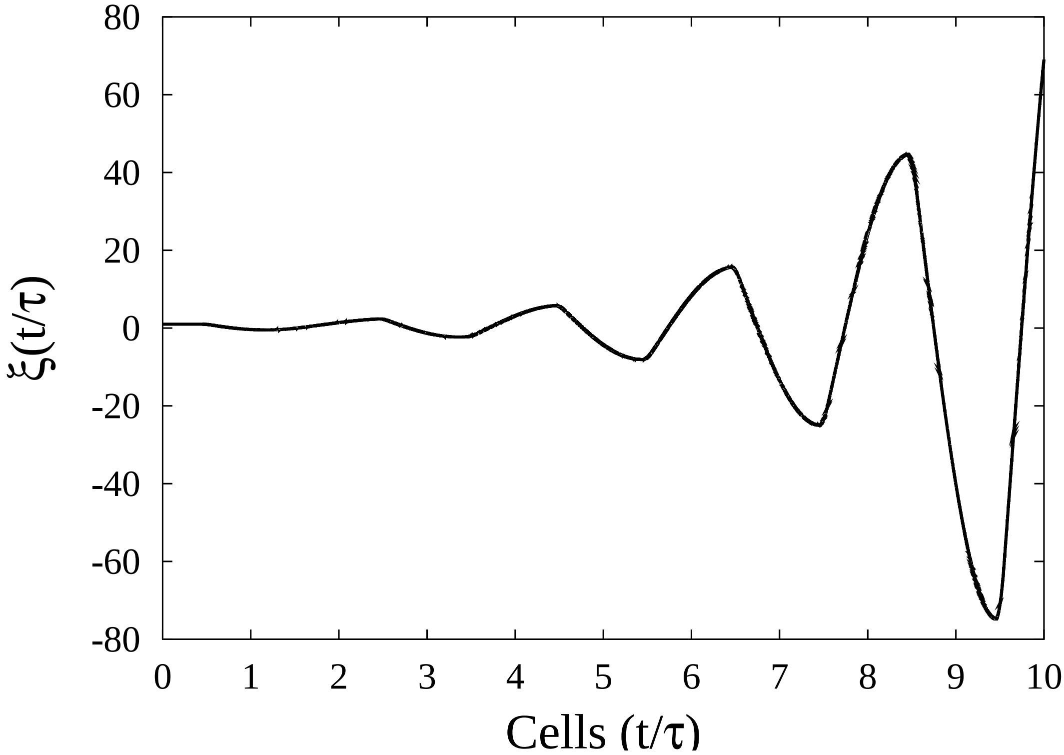

Figure 1.5: $\xi(t)$ as unstable solution of (1.82) for $\sigma_0 = 60°$, $\sigma = 15°$. τ denotes the focusing period common to all three directions.

Figs. 1.4 and 1.5 show the function $\xi(t)$ as the result of numerical integrations of the coupled set (1.84) and (1.85). The second-order moments — denoted by the angle brackets — and the field energy function $W(t)$ were taken from simulations of a fictitious three-dimensional anisotropic focusing lattice that is described by the Hamiltonian (1.79) with the potential (1.80). The simulation leading to Fig. 1.4 was performed at the zero-current tune of $\sigma_0 = 45°$, and a space-charge depressed tune of $\sigma = 9°$ in each direction. As a result of various simulations, we found that $\xi(t)$ becomes unstable for $\sigma_0 \geq 60°$. Furthermore, it turned out that this limit value for an unstable evolution of $\xi(t)$ decreases as the field energy $W(t)$ increases. A case with a growing amplitude of $\xi(t)$ is displayed in Fig. 1.5 for a beam propagating under the conditions of a zero-current tune of $\sigma_0 = 60°$ and the depressed tune of $\sigma = 15°$. In agreement with earlier studies on high current beam transport [23], the simulation results show that the beam moments remain bounded under these conditions. This means that an instability of $\xi(t)$ is *not* necessarily associated with an instability of the beam moments. Nevertheless, the phase-space planes of constant I become more and more distorted as $\xi(t)$ and its derivatives diverge. This may indicate a transition from a regular to a chaotic motion of the beam particles.

1.5 Checking the overall accuracy of numerical simulations of Hamiltonian systems

The conserved quantity I that has been shown to exist for explicitly time-dependent Hamiltonian systems can be used to test the results of numerical simulations of such systems [24, 25]. As already stated in Sec. 1.3 for the general form of the invariant I, Eq. (1.83) embodies a time integral of (1.82) if the system's time evolution is *strictly* consistent with the equations of motion (1.81). In the ideal case, i.e. if no numerical inaccuracies were included in a computer simulation

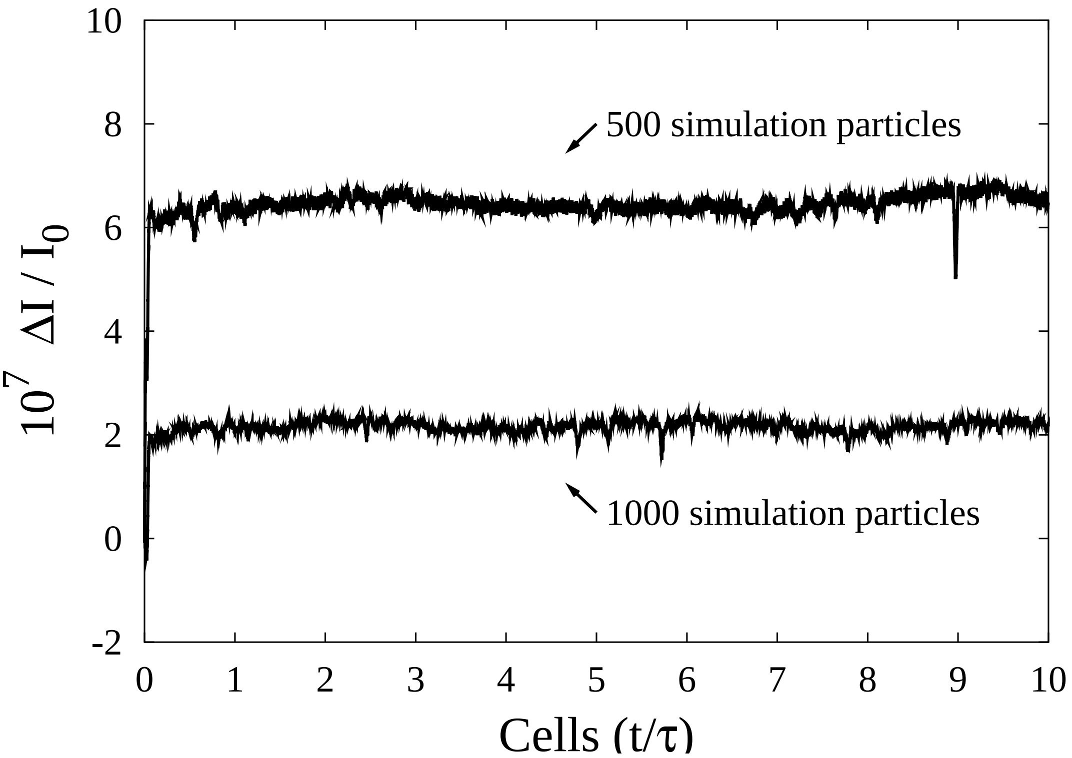

Figure 1.6: Relative invariant error $\Delta I/I_0$ for three-dimensional simulations of a charged particle beam with different numbers of macro-particles.

of a system governed by (1.79), and no numerical errors were added performing the subsequent integration of (1.82), we would not see any deviation $\Delta I/I_0$ calculating the invariant (1.83) as a function of time.

Of course, we can never avoid numerical errors in computer simulations of dynamical systems because of the generally limited accuracy of numerical methods. For the same reason, the numerical integration of Eq. (1.82) is also associated with a specific finite error tolerance. Under these circumstances, the quantity I as given by Eq. (1.83) — with $\xi(t)$, $\dot{\xi}(t)$, and $\ddot{\xi}(t)$ following from (1.82) — can no longer be expected to be *exactly* constant. Both numerical tasks — the numerical integration of the equations of motion (1.81), and the subsequent numerical integration of Eq. (1.82) contribute to a non-vanishing $\Delta I/I_0$ along the integration time span. Nevertheless, since both tasks do not depend on each other with respect to their specific error tolerances, we can regard the obtained $\Delta I/I_0$ curve as a cross-check of both numerical methods. Since the error tolerance for the numerical integration of Eq. (1.82) is a known property of the underlying algorithm, we can estimate from $\Delta I(t)/I_0$ the error tolerance integrating the equations of motion (1.81).

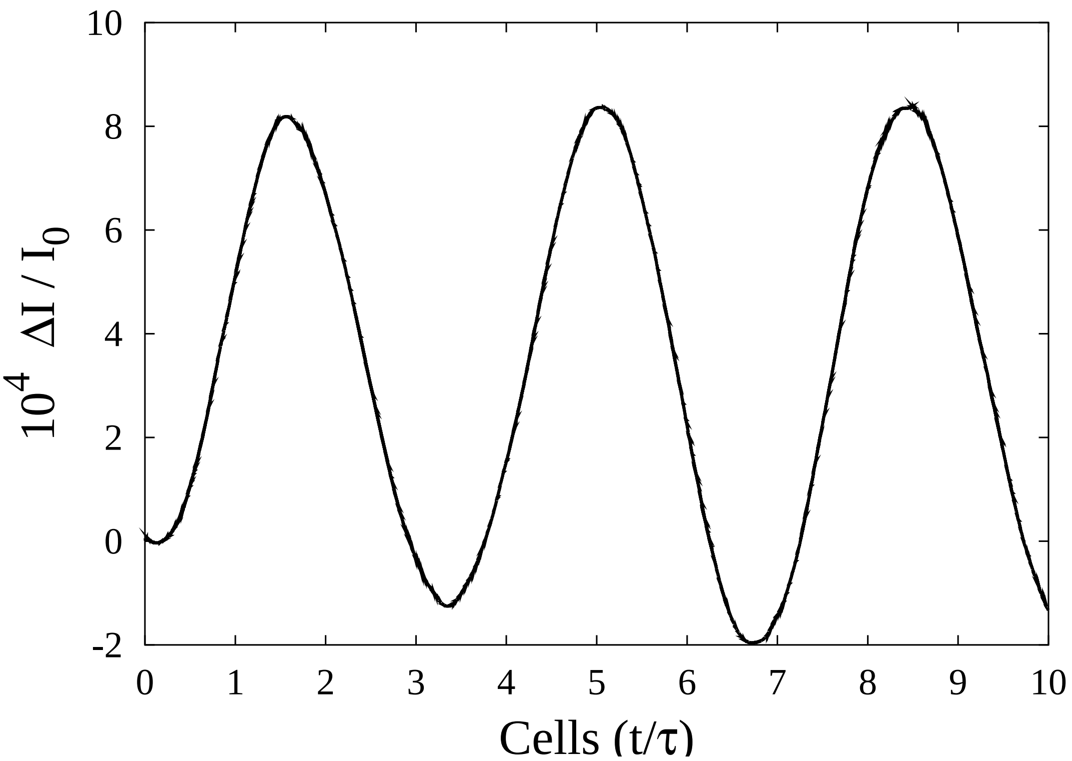

Figure 1.7: Relative invariant error $\Delta I/I_0$ for a three-dimensional simulation of a charged particle beam with 5 %-error in the space-charge force calculations.

Fig. 1.6 displays two examples of curves of relative deviations $\Delta I/I_0$ from the invariant (1.83) for numerical simulations of a charged particle beam. The function $\xi(t)$ and its derivatives that were used to calculate I were obtained from a numerical integration of Eq. (1.82) — or equivalently from the coupled set (1.84) and (1.85). The time-dependent coefficients of (1.82), namely the second beam moments and the field energy $W(t)$, had been determined before from three-dimensional simulations of charged particle beams propagating through a linear focusing lattice with non-negligible Coulomb interaction, as described by the potential function (1.80). As expected, the residual deviation $\Delta I/I_0$ depends on the number of macro-particles used in the simulation.

For a comparison, the corresponding deviation is plotted in Fig. 1.7 for a simulation with a systematic 5 %-error in the space-charge force calculations. We now find a relative deviation $\Delta I/I_0$ in the order of 10^{-3}, hence three orders of magnitude larger than the previous case with no artificial space-charge force error. By comparing simulation runs with different parameters, such as the number of macro-particles, the time step size, details of the numerical algorithm used to integrate the equations of motion, we may straightforwardly check whether the overall accuracy of our particular simulation has been improved.

1.6 More general symmetry transformations: infinitesimal canonical transformations

1.6.1 General conditions for infinitesimal canonical transformations

In the extended phase space, the generating function F_2 of an infinitesimal canonical transformation is given by

$$F_2(\vec{q},\vec{p}\,',t,\mathcal{H}') = \sum_{i=1}^{n} q_i p_i' - t\mathcal{H}' - \varepsilon G(\vec{q},\vec{p},t,\mathcal{H})\,, \tag{1.87}$$

with ε an infinitesimal parameter, and $G(\vec{q},\vec{p},t,\mathcal{H})$ the function that characterizes the deviation of the canonical transformation from the identity. Since the transformation generated by (1.87) is infinitesimal, to first order in ε the old (unprimed) canonical variables can be used calculating the derivatives of $G(\vec{q},\vec{p},t,\mathcal{H})$. From the transformation rules (1.14), we thus find

$$q_i' = q_i - \varepsilon\,\frac{\partial G}{\partial p_i}\,,\quad p_i' = p_i + \varepsilon\,\frac{\partial G}{\partial q_i}\,,\quad t' = t + \varepsilon\,\frac{\partial G}{\partial \mathcal{H}}\,,\quad \mathcal{H}' = \mathcal{H} - \varepsilon\,\frac{\partial G}{\partial t}\,. \tag{1.88}$$

The variation of the function $G(\vec{q},\vec{p},t,\mathcal{H})$ is given by

$$\delta G = \sum_{i=1}^{n}\left(\frac{\partial G}{\partial q_i}\delta q_i + \frac{\partial G}{\partial p_i}\delta p_i\right) + \frac{\partial G}{\partial t}\delta t + \frac{\partial G}{\partial \mathcal{H}}\delta\mathcal{H}\,.$$

Inserting Eqs. (1.88), we get

$$\delta G = \varepsilon\left\{\sum_{i=1}^{n}\left(-\frac{\partial G}{\partial q_i}\frac{\partial G}{\partial p_i} + \frac{\partial G}{\partial p_i}\frac{\partial G}{\partial q_i}\right) + \frac{\partial G}{\partial t}\frac{\partial G}{\partial \mathcal{H}} - \frac{\partial G}{\partial \mathcal{H}}\frac{\partial G}{\partial t}\right\} = 0\,, \tag{1.89}$$

which means that $G(\vec{q},\vec{p},t,\mathcal{H})$ remains invariant by virtue of the canonical transformation. In other words, the infinitesimal part of (1.87) itself provides the quantity that is conserved performing the canonical transformation generated by (1.87).

Moreover, the variation $\delta\widetilde{H} = \widetilde{H}' - \widetilde{H}$ of the Hamiltonian $\widetilde{H}$ under the action of the infinitesimal canonical transformation (1.88) must also vanish, as stated by Eq. (1.11)

$$\begin{aligned}\delta\widetilde{H} &= \varepsilon\left[\sum_{i=1}^{n}\left(\frac{\partial\widetilde{H}}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial\widetilde{H}}{\partial p_i}\frac{\partial G}{\partial q_i}\right) - \frac{\partial\widetilde{H}}{\partial t}\frac{\partial G}{\partial \mathcal{H}} + \frac{\partial\widetilde{H}}{\partial \mathcal{H}}\frac{\partial G}{\partial t}\right]\\ &= 0\,.\end{aligned} \tag{1.90}$$

Equation (1.90) can be regarded as a condition to be satisfied by the constituent part of the generating function (1.87) in order to comply with Eq. (1.11), hence to actually represent a canonical transformation in the extended phase space. Inserting the canonical equations (1.7), we find that Eq. (1.90) implies

$$\frac{dG}{ds} = 0\,. \tag{1.91}$$

Therefore, the transformation (1.88) that is induced by G is canonical if and only if $dG/ds = 0$. This means that G must constitute an integral of motion along the system's phase-space trajectory. Invariants of that kind are thus constituted by *all* functions of the extended phase-space variables that are contained in the generating function of an infinitesimal canonical transformation in the extended phase space. As the number of invariants that can be constructed that way is not limited, we cannot expect that a physical meaning can be attributed to each particular invariant.

We now define a general time-dependent infinitesimal symmetry mapping that is supposed to be consistent with (1.88)

$$t' = \quad t+\delta t = t \quad +\varepsilon\,\xi(t) \tag{1.92}$$
$$q_i'(t') = q_i(t)+\delta q_i = q_i(t)+\varepsilon\,\eta_i(\vec{q},\vec{p},t) \tag{1.93}$$
$$p_i'(t') = p_i(t)+\delta p_i = p_i(t)+\varepsilon\,\pi_i(\vec{q},\vec{p},t)\,. \tag{1.94}$$

Comparing the partial derivatives of the function $G(\vec{q},\vec{p},t,\mathcal{H})$, as given by Eqs. (1.88), with the Ansatz (1.92), (1.93), and (1.94) for the the time-dependent symmetry mapping, we find

$$\frac{\partial G}{\partial q_i} = \pi_i\,, \qquad \frac{\partial G}{\partial p_i} = -\eta_i\,, \qquad \frac{\partial G}{\partial \mathcal{H}} = \xi(t)\,. \tag{1.95}$$

Consequently, η_i and π_i cannot be independent of each other. Following from the mixed second derivatives $\partial^2 G/\partial q_i \partial p_j$ of G, the functions η_j and π_i must satisfy

$$\frac{\partial \pi_i}{\partial p_j} = -\frac{\partial \eta_j}{\partial q_i}\,, \quad i,j = 1,\ldots,n\,. \tag{1.96}$$

Again, the condition for a conserved Hamiltonian $\delta\widetilde{H} = 0$ may be written as the requirement of Eq. (1.91) for a vanishing total s-derivative of $G(\vec{q},\vec{p},t,\mathcal{H})$. By virtue of Eqs. (1.7), (1.8), and (1.9), the condition $dG/ds = 0$ writes in terms of the original Hamiltonian H

$$\frac{dG}{ds} = \frac{dt}{ds}\left[\frac{\partial G}{\partial t} + \xi(t)\frac{\partial H}{\partial t} + \sum_{i=1}^{n}\left(\pi_i\frac{\partial H}{\partial p_i} + \eta_i\frac{\partial H}{\partial q_i}\right)\right] = 0\,. \tag{1.97}$$

As dt/ds is generally non-zero, the expression in brackets must vanish in order for G to comply with the condition of Eq. (1.11) for canonical transformations.

The constituents η_i, π_i, and ξ of the point transformation (1.92), (1.93), and (1.94) may be regarded as Ansatz functions that must be chosen appropriately to emerge from a common characteristic function G according to Eqs. (1.95). This defines a procedure to construct a generating function F_2 of a canonical transformation in the extended phase space. As the total s-derivative of the characteristic part G of this generating function vanishes by virtue of Eq. (1.91), we thereby encounter an integral of motion of the underlying dynamical system. Replacing $\mathcal{H}$ according to Eq. (1.4), this integral of motion can always be expressed equivalently in terms of the conventional phase-space variables $\vec{q}$, $\vec{p}$, and t.

The quantities δq_i and δp_i in (1.93) and (1.94) stand for the variation of the canonical variables as a result of the canonical transformation at *different* instants of time. In order to separate the time shift from the coordinate transformation rules, we split (1.93) and (1.94) into the coordinate transformation part at fixed time t', and the time shift part according to

$$\delta q_i = \varepsilon\eta_i = \Big[q_i'(t') - q_i(t')\Big] + \Big[q_i(t') - q_i(t)\Big]$$
$$\delta p_i = \varepsilon\pi_i = \Big[p_i'(t') - p_i(t')\Big] + \Big[p_i(t') - p_i(t)\Big]\,.$$

Since we are dealing with an *infinitesimal* transformation, the right brackets may be identified without loss of generality with the first order term of a Taylor series

$$q_i(t') - q_i(t) = \dot{q}_i\,\delta t\,, \qquad p_i(t') - p_i(t) = \dot{p}_i\,\delta t\,.$$

Solving for the terms in the left brackets, we finally have in conjunction with (1.92)

$$q_i'(t') - q_i(t') = \varepsilon\left(\eta_i(\vec{q},\vec{p},t) - \xi(t)\,\dot{q}_i\right) \tag{1.98}$$
$$p_i'(t') - p_i(t') = \varepsilon\left(\pi_i(\vec{q},\vec{p},t) - \xi(t)\,\dot{p}_i\right)\,. \tag{1.99}$$

With the requirement that the functions $\eta_i = \eta_i(\vec{q},\vec{p},t)$ and $\pi_i = \pi_i(\vec{q},\vec{p},t)$ fulfill condition (1.96), the coupled set of equations (1.92), (1.98), and (1.99) provides the general form of the transformation rules for infinitesimal canonical transformations in the extended phase space. In the following section, we will specialize this general transformation for a specific class of Hamiltonian systems. The invariant G can then be worked out in explicit form making use of (1.95). The conditional equation for $\xi(t)$ is finally established by Eq. (1.97).

1.6.2 Example 1: general time-dependent potential

We again consider the n-degree-of-freedom system of particles moving in an explicitly time-dependent potential $V(\vec{q},t)$ with time-dependent damping forces proportional to the velocity, as described by the Hamiltonian (1.17). In the following, we work out the invariant G of the Hamiltonian system (1.17) that corresponds to the symmetry mapping (1.92), (1.98), and (1.99) with the more specific functions $\eta_i = \eta_i(q_i,t)$ and $\pi_i = \pi_i(q_i,p_i,t)$

$$q_i'(t') - q_i(t') = \varepsilon\left(\eta_i(q_i,t) \qquad - \xi(t)\,\dot{q}_i\right) \tag{1.100}$$

$$p_i'(t') - p_i(t') = \varepsilon\left(\pi_i(q_i,p_i,t) - \xi(t)\,\dot{p}_i\right). \tag{1.101}$$

We choose the connection between Eqs. (1.100) and (1.101) to be established by the first canonical equation of (1.18)

$$p_i'(t') - p_i(t') = e^{F(t)}\frac{d}{dt}\left(q_i' - q_i\right)\Bigg|_{t'} = \varepsilon\, e^{F(t)}\frac{d}{dt}\left(\eta_i(q_i,t) - \xi(t)\,\dot{q}_i\right).$$

Hereby, we determine the invariant G to represent a conserved quantity along the system's evolution in time. With Eq. (1.101) and the first canonical equation of (1.18), we then obtain for π_i

$$\pi_i(q_i,p_i,t) = \left(\frac{\partial\eta_i}{\partial q_i} - \dot{\xi}(t) + \xi(t)f(t)\right)p_i + \frac{\partial\eta_i}{\partial t}e^{F(t)}. \tag{1.102}$$

The function $\eta_i(q_i,t)$ can now be determined from Eq. (1.102) with the help of Eq. (1.96)

$$\frac{\partial\eta_i}{\partial q_i} = \tfrac{1}{2}\dot{\xi}(t) - \tfrac{1}{2}\xi(t)\,f(t)\,, \tag{1.103}$$

which can be integrated to give

$$\eta_i(q_i,t) = \tfrac{1}{2}q_i\left(\dot{\xi} - \xi f\right) + \psi_i(t)\,. \tag{1.104}$$

Herein, $\psi_i(t)$ denotes an arbitrary function of time only. Inserting Eq. (1.103) and the partial time derivative of Eq. (1.104) into Eq. (1.102), we eliminate its dependence on η_i

$$\pi_i(q_i,p_i,t) = -\tfrac{1}{2}p_i\left(\dot{\xi} - \xi f\right) + \tfrac{1}{2}q_i e^{F(t)}\left(\ddot{\xi} - \dot{\xi}f - \xi\dot{f}\right) + \dot{\psi}_i e^{F(t)}\,. \tag{1.105}$$

Now that η_i and π_i are specified by Eqs. (1.104) and (1.105), respectively, the invariant $G(\vec{q},\vec{p},t)$ in its conventional phase-space representation can be deduced from its partial derivatives (1.95)

$$\begin{aligned} G(\vec{q},\vec{p},t) = \xi\,H - \tfrac{1}{2}\left(\dot{\xi} - \xi\,f\right)\sum_{i=1}^{n} q_i\,p_i + \tfrac{1}{4}e^{F(t)}\left(\ddot{\xi} - \dot{\xi}f - \xi\dot{f}\right)\sum_{i=1}^{n} q_i^2 \\ + \sum_{i=1}^{n}\left(\dot{\psi}_i\,q_i\,e^{F(t)} - \psi_i\,p_i\right). \end{aligned} \tag{1.106}$$

The functions $\xi(t)$ and $\psi_i(t)$ are determined by the condition (1.97) for $G(\vec{q},\vec{p},t)$ to yield an invariant. Calculating the partial time derivative of Eq. (1.106) and making use of the explicit form of the Hamiltonian (1.17), Eq. (1.97) leads to the following linear differential equations for $\xi(t)$ and $\psi_i(t)$

$$\dddot{\xi}\sum_{i=1}^{n} q_i^2 + 4\dot{\xi}\left[V(\vec{q},t) + \tfrac{1}{2}\sum_{i=1}^{n} q_i\frac{\partial V}{\partial q_i} - \tfrac{1}{2}\left(\dot{f} + \tfrac{1}{2}f^2\right)\sum_{i=1}^{n} q_i^2\right]$$
$$+ 4\xi\left[\frac{\partial V}{\partial t} + f\left(V(\vec{q},t) - \tfrac{1}{2}\sum_{i=1}^{n} q_i\frac{\partial V}{\partial q_i}\right) - \tfrac{1}{4}\left(\ddot{f} + f\dot{f}\right)\sum_{i=1}^{n} q_i^2\right] = 0\,, \tag{1.107}$$

$$\ddot{\psi}_i\, q_i - \psi_i\, \ddot{q}_i + \left(\dot{\psi}_i\, q_i - \psi_i\, \dot{q}_i\right) f = 0\,, \qquad i = 1,\ldots,n\,. \tag{1.108}$$

Since the $\psi_i(t)$ are arbitrary functions that do not depend on $\xi(t)$, the respective expressions must vanish separately. We thus obtain distinct differential equations for $\xi(t)$ and $\psi_i(t)$, as given by Eqs. (1.107) and (1.108). We observe that Eq. (1.107) agrees with the conditional equation (1.27) for $\xi(t)$ derived in the context of the finite canonical transformation of the Hamiltonian (1.17).

The total time derivative of the ψ_i-terms in Eq. (1.106) vanish because of Eq. (1.108). Consequently, the related sum in Eq. (1.106) provides a separate invariant

$$\sum_{i=1}^{n}\left(\dot{\psi}_i(t)\, q_i\, e^{F(t)} - \psi_i(t)\, p_i\right) = \widetilde{I} = \text{const.}\,,$$

which means that the invariant G can be written as a sum of two invariants

$$G(\vec{q},\vec{p},t) = I + \widetilde{I}\,.$$

The terms associated with the function $\xi(t)$ thus form a separate invariant I

$$I = \xi\, H(\vec{q},\vec{p},t) - \tfrac{1}{2}\left(\dot{\xi} - \xi\, f\right)\sum_{i=1}^{n} q_i\, p_i + \tfrac{1}{4}e^{F(t)}\left(\ddot{\xi} - \dot{\xi}f - \xi\dot{f}\right)\sum_{i=1}^{n} q_i^2\,,$$

which again agrees with invariant of Eq. (1.29).

The invariant (1.106), together with the conditional equations (1.107) and (1.108) for $\xi(t)$ and the $\psi_i(t)$, have been shown to follow equivalently from Noether's theorem. We conclude that the particular subset of the general canonical symmetry transformation (1.98) and (1.99), defined by Eqs. (1.100) and (1.101), together with the conditions (1.95) and (1.96), is equivalent to the Noether symmetry transformation (1.30). Hence, the general form canonical transformations (1.92), (1.98), and (1.99) — wherein η_i also depends on the canonical momenta — allows to isolate more general symmetries as compared to Noether's approach. This will be demonstrated with an example in the following section.

1.6.3 Example 2: time-dependent anisotropic two-dimensional harmonic oscillator

In this example, we perform canonical symmetry mappings for the two-dimensional system of a time-dependent anisotropic oscillator without damping in order to derive invariants for this system. Its Hamiltonian is given by

$$H = \sum_{i=1}^{2} H_i\,, \qquad H_i = \tfrac{1}{2}p_i^2 + \tfrac{1}{2}\omega_i^2(t)\, q_i^2\,, \tag{1.109}$$

leading to the canonical equations

$$\dot{q}_i = p_i\,, \qquad \dot{p}_i = -\omega_i^2(t)\, q_i\,, \qquad i = 1,2\,. \tag{1.110}$$

Symmetry mapping 1

For this first symmetry mapping, we again use the actual first canonical equation $p_i = \dot{q}_i$ in order to establish the relation between Eqs. (1.98) and (1.99)

$$p_i'(t') - p_i(t') = \frac{d}{dt}\Big(q_i' - q_i\Big)\bigg|_{t'} .$$

Inserting Eqs. (1.99), the expression for $\pi_i = \pi_i(q_i, p_i, t)$ is obtained as

$$\pi_i(q_i, p_i, t) = \left(\frac{\partial \eta_i}{\partial q_i} - \dot{\xi}(t)\right) p_i + \frac{\partial \eta_i}{\partial t} . \tag{1.111}$$

The function $\eta_i = \eta_i(q_i, t)$ is immediately found applying (1.96) on (1.111)

$$\eta_i = \tfrac{1}{2}\dot{\xi}(t)\, q_i + \psi_i(t) . \tag{1.112}$$

We can now eliminate the η_i-dependent terms in (1.111)

$$\pi_i(q_i, p_i, t) = \tfrac{1}{2}\ddot{\xi}(t)\, q_i - \tfrac{1}{2}\dot{\xi}(t)\, p_i + \dot{\psi}_i(t) \tag{1.113}$$

and deduce the invariant $G(\vec{q}, \vec{p}, t)$ from its partial derivatives (1.112) and (1.113) according to (1.95)

$$G = \xi(t)H - \tfrac{1}{2}\dot{\xi}(t)\sum_i q_i p_i + \tfrac{1}{4}\ddot{\xi}(t)\sum_i q_i^2 + \sum_i \big(\dot{\psi}_i q_i - \psi_i p_i\big) . \tag{1.114}$$

As expected, the invariant G represents the specialization of the general invariant (1.29) for two dimensions with zero damping functions $(F(t) = f(t) = 0)$. The function $\xi(t)$ is given as a solution of the linear third-order differential equation

$$\sum_i \Big[\dddot{\xi}(t) + 4\dot{\xi}(t)\,\omega_i^2(t) + 4\xi(t)\,\omega_i\dot{\omega}_i\Big] q_i^2(t) = 0 , \tag{1.115}$$

which follows with (1.109) from (1.97). In contrast to the equations of motion (1.110), the two degrees of freedom are coupled in Eq. (1.115) since the function $\xi(t)$ depends on all particle coordinates $q_i(t)$.

For the particular case of a time-independent two-dimensional harmonic oscillator ($\omega_i =$ const.), the terms proportional to $\xi(t)$ vanish

$$\sum_i \Big[\dddot{\xi}(t) + 4\omega_i^2\,\dot{\xi}(t)\Big] q_i^2(t) = 0 . \tag{1.116}$$

Then, $\xi(t) \equiv 1$ is a solution of (1.116), and the ξ-dependent part I_0 of the invariant (1.114) represents the conserved total energy

$$I_0 = H = \sum_i H_i .$$

On the other hand, Eq. (1.116) also admits solutions $\xi(t) \neq$ const. Due to the explicit time-dependence of $q_i(t)$, Eq. (1.116) then represents a linear second-order differential equation for $\zeta(t) \equiv \dot{\xi}(t)$ with periodic coefficients, which can be written equivalently in the standard form of a Hill equation

$$\ddot{\zeta} + \omega^2(t)\,\zeta = 0 , \qquad \text{with} \qquad \omega^2(t) = \sum_i 4\omega_i^2 q_i^2 \Big/ \sum_i q_i^2 .$$

For the isotropic case ($\omega_1 = \omega_2$), we have $\omega(t) = 2\omega_1 = \text{const}$. Then, the solutions $\xi(t)$ of the auxiliary equation (1.116) are always stable. In the anisotropic case ($\omega_1 \neq \omega_2$), the solutions $\xi(t)$ may become unstable, depending on the amplitude of $\omega^2(t)$, hence the strength of the system's anisotropy. This demonstrates a general feature of the invariant (1.29), and hence the particular invariant (1.114): even in the case of an *autonomous* system, the solutions of the auxiliary equation with $\xi(t) \neq \text{const}$. depend on the vector of particle trajectories $\vec{q}(t)$. The coupling of the auxiliary equation to the equations of motion cancels solely for isotropic linear systems.

Symmetry mapping 2

We now discuss the way to obtain further non-trivial invariants for this example case. We can, for example, restrict the time-dependent symmetry mappings (1.93) and (1.94) to the canonical variables q_1 and p_1 only, leaving q_2 and p_2 unchanged. Taking η_1 and π_1 from (1.112) and (1.113), we define the infinitesimal transformation by

$$\begin{aligned} \eta_1 &= -\frac{\partial G}{\partial p_1} = \tfrac{1}{2}\dot{\xi} q_1 + \psi_1 & \eta_2 &= 0 \\ \pi_1 &= \quad \frac{\partial G}{\partial q_1} = \tfrac{1}{2}\ddot{\xi} q_1 - \tfrac{1}{2}\dot{\xi} p_1 + \dot{\psi}_1 & \pi_2 &= 0\,. \end{aligned} \tag{1.117}$$

The function $G(q_1, p_1, t)$ whose partial derivatives (1.95) are given by (1.117) is

$$G(q_1, p_1, t) = \xi H - \tfrac{1}{2}\dot{\xi} q_1 p_1 + \tfrac{1}{4}\ddot{\xi} q_1^2 + \dot{\psi}_1 q_1 - \psi_1 p_1\,. \tag{1.118}$$

The conditional equation for $\xi(t)$ which must be fulfilled to ensure the invariance of (1.118) can be derived from Eq. (1.97)

$$\frac{\partial G}{\partial t} = -\frac{\partial (H_1 + H_2)}{\partial t}\xi(t) - \frac{\partial H}{\partial q_1}\eta_1 - \frac{\partial H}{\partial p_1}\pi_1\,.$$

Together with the partial time derivative of (1.118), we get inserting the functions from Eq. (1.117)

$$q_1\big(\ddot{\psi}_1 + \omega_1^2 \psi_1\big) = -\tfrac{1}{4} q_1^2 \big(\dddot{\xi} + 4\dot{\xi}\omega_1^2 + 4\xi\omega_1\dot{\omega}_1\big) - \frac{d}{dt}\big(\xi H_2\big)\,.$$

Using the equation of motion $\ddot{q}_1 = -\omega_1^2 q_1$, we find that the expression on the l.h.s. is the total time derivative of the function $\dot{\psi}_1 q_1 - \psi_1 \dot{q}_1$. Also the third order differential expression on the r.h.s. can be expressed as a total time derivative

$$\frac{d}{dt}\big(\dot{\psi}_1 q_1 - \psi_1 \dot{q}_1\big) + \frac{d}{dt}\big(\xi H_2\big) = -\tfrac{1}{4}\frac{q_1^2}{\xi}\frac{d}{dt}\big(\ddot{\xi}\xi - \tfrac{1}{2}\dot{\xi}^2 + 2\omega_1^2\xi^2\big)\,. \tag{1.119}$$

We are free to choose the function $\psi_1(t)$ in a way to render the l.h.s. of Eq. (1.119) zero. Then, the r.h.s. of (1.119) yields the conditional equation for $\xi(t)$

$$\ddot{\xi}\xi - \tfrac{1}{2}\dot{\xi}^2 + 2\omega_1^2(t)\xi^2 = c = \text{const.} \tag{1.120}$$

The l.h.s. of (1.119) can be integrated

$$\widetilde{I} = \dot{\psi}_1 q_1 - \psi_1 \dot{q}_1 + \xi H_2$$

and inserted into Eq. (1.118)

$$G - \widetilde{I} = I_1 = \xi\big(\tfrac{1}{2}p_1^2 + \tfrac{1}{2}\omega_1^2 q_1^2\big) + \xi H_2 - \tfrac{1}{2}\dot{\xi} q_1 \dot{q}_1 + \tfrac{1}{4}\ddot{\xi} q_1^2 - \xi H_2\,.$$

It is interesting to observe that terms related to the part H_2 of the Hamiltonian, which were not affected by the symmetry mappings (1.117), cancel exactly. The invariant I_1 thus finally reads

$$I_1 = \tfrac{1}{2}\xi(t)\big(p_1^2 + \omega_1^2 q_1^2\big) - \tfrac{1}{2}\dot{\xi}(t)\, q_1 p_1 + \tfrac{1}{4}\ddot{\xi}(t)\, q_1^2 \,. \tag{1.121}$$

Calculating the total time derivative of (1.121) and using the equations of motion (1.110) it can easily be shown that I_1 is indeed an invariant, provided $\xi(t)$ satisfies Eq. (1.120).

Equation (1.120) is the differential equation for the function $\xi(t)$ in the case of the time-dependent one-dimensional oscillator (cf also Eq. (1.66) for vanishing damping coefficient $f = 0$). For the time-independent case ($\omega_1 =$ const.), Eq. (1.120) allows the constant solution $\xi(t) \equiv 1$, and the invariant I_1 agrees with the conserved partial energy $I_1 = H_1$.

Correspondingly, an invariant I_2 can readily be derived

$$I_2 = \tfrac{1}{2}\xi_2(t)\big(p_2^2 + \omega_2^2 q_2^2\big) - \tfrac{1}{2}\dot{\xi}_2(t)\, q_2 p_2 + \tfrac{1}{4}\ddot{\xi}_2(t)\, q_2^2 \,,$$

where $\xi_2(t)$ now fulfills the differential equation similar to (1.120)

$$\ddot{\xi}_2\xi_2 - \tfrac{1}{2}\dot{\xi}_2^2 + 2\omega_2^2(t)\xi_2^2 = c_2 = \text{const.}$$

For the time-independent oscillator, this invariant corresponds to $I_2 = H_2$.

Symmetry mapping 3

As has been pointed out in Sec. 1.6.1, all functions $\eta_i(\vec{q},\vec{p},t)$ and $\pi_i(\vec{q},\vec{p},t)$ that fulfill the invariance condition (1.96) for the Poisson brackets can be used in the infinitesimal canonical transformation. In the case of a harmonic two-dimensional oscillator, the corresponding invariants represent its well-known SU(2)-symmetry [26].

The infinitesimal canonical transformation generated by the symmetry mapping

$$\begin{aligned} \eta_1 &= -\frac{\partial G}{\partial p_1} = \tfrac{1}{2}\dot{\xi} q_1 - \xi p_2 & \eta_2 &= -\frac{\partial G}{\partial p_2} = \tfrac{1}{2}\dot{\xi} q_2 - \xi p_1 \\ \pi_1 &= \frac{\partial G}{\partial q_1} = -\tfrac{1}{2}\dot{\xi} p_1 + \xi\omega_1\omega_2 q_2 & \pi_2 &= \frac{\partial G}{\partial q_2} = -\tfrac{1}{2}\dot{\xi} p_2 + \xi\omega_1\omega_2 q_1 \end{aligned} \tag{1.122}$$

satisfies condition (1.96) for Poisson brackets and leads to the invariant

$$I_3 = \xi(t)H - \tfrac{1}{2}\dot{\xi}(t)\big(q_1 p_1 + q_2 p_2\big) + \xi(t)\big(p_1 p_2 + \omega_1\omega_2 q_1 q_2\big)\,. \tag{1.123}$$

Requiring the total time derivative dI_3/dt to vanish, and using the equations of motion (1.110), the conditional differential equation for $\xi(t)$ can be determined

$$\begin{aligned} &\ddot{\xi}(t)\big[q_1 p_1 + q_2 p_2\big] - 2\dot{\xi}(t)\,\big[\omega_1^2 q_1^2 + \omega_2^2 q_2^2 + \omega_1\omega_2 q_1 q_2 + p_1 p_2\big] \\ &-2\xi(t)\big[\,\omega_1\omega_2(q_1 p_2 + q_2 p_1) - \omega_1^2 q_1 p_2 - \omega_2^2 q_2 p_1 + \\ &\qquad \omega_1\dot{\omega}_1 q_1^2 + \omega_2\dot{\omega}_2 q_2^2 + q_1 q_2\big(\dot{\omega}_1\omega_2 + \omega_1\dot{\omega}_2\big)\big] = 0\,. \end{aligned} \tag{1.124}$$

For the time-independent isotropic harmonic two-dimensional oscillator ($\omega_1 = \omega_2 = \omega =$ const.), the coefficient of $\xi(t)$ in (1.124) vanishes, and $\xi(t) \equiv 1$ is a solution of the differential equation. Since the Hamiltonian is a conserved quantity in this case, we obtain an invariant

$$I_3' = p_1 p_2 + \omega^2 q_1 q_2\,. \tag{1.125}$$

Symmetry mapping 4

For the symmetry mapping

$$\begin{aligned} \eta_1 &= -\frac{\partial G}{\partial p_1} = \tfrac{1}{2}\dot{\xi} q_1 + \xi\omega_2 q_2 \quad & \eta_2 &= -\frac{\partial G}{\partial p_2} = \tfrac{1}{2}\dot{\xi} q_2 - \xi\omega_1 q_1 \\ \pi_1 &= \frac{\partial G}{\partial q_1} = -\tfrac{1}{2}\dot{\xi} p_1 + \xi\omega_1 p_2 \quad & \pi_2 &= \frac{\partial G}{\partial q_2} = -\tfrac{1}{2}\dot{\xi} p_2 - \xi\omega_2 p_1 \end{aligned} \tag{1.126}$$

we can write down an infinitesimal canonical transformation that leads to the invariant

$$I_4 = \xi(t)H - \tfrac{1}{2}\dot{\xi}(t)\left(q_1p_1 + q_2p_2\right) + \xi(t)\left(\omega_1 q_1 p_2 - \omega_2 q_2 p_1\right) . \tag{1.127}$$

In a similar manner to Sec. 1.6.3, we obtain for the time-independent isotropic harmonic oscillator case the invariant

$$I_4' = \omega(q_1p_2 - q_2p_1) . \tag{1.128}$$

Symmetry mapping 5

Finally, the symmetry mapping

$$\begin{aligned} \eta_1 &= -\frac{\partial G}{\partial p_1} = \tfrac{1}{2}\dot{\xi} q_1 + \xi p_1 \quad & \eta_2 &= -\frac{\partial G}{\partial p_2} = \tfrac{1}{2}\dot{\xi} q_2 - \xi p_2 \\ \pi_1 &= \frac{\partial G}{\partial q_1} = -\tfrac{1}{2}\dot{\xi} p_1 - \xi\omega_1^2 q_1 \quad & \pi_2 &= \frac{\partial G}{\partial q_2} = -\tfrac{1}{2}\dot{\xi} p_2 + \xi\omega_2^2 q_2 \end{aligned} \tag{1.129}$$

leads to the corresponding invariant

$$I_5 = \xi(t)H - \tfrac{1}{2}\dot{\xi}(t)\left[q_1p_1 + q_2p_2\right] + \tfrac{1}{2}\xi(t)\left[p_2^2 + \omega_2^2 q_2^2 - p_1^2 - \omega_1^2 q_1^2\right] , \tag{1.130}$$

and

$$I_5' = H_2 - H_1 . \tag{1.131}$$

1.7 General aspects of invariants for non-linear time-dependent systems

Following a conventional understanding, the search for invariants is motivated by the idea to reduce the order of the system's equations of motion. In the extreme case, this strategy would mean to construct the solution of a given dynamical system by finding all its invariants.

Unfortunately, this scheme does not work in practice. Apart from particular cases — mostly associated with potentials that are of no practical interest — all attempts to solve a problem by gradually reducing its order usually fail. This is particularly true for all problems of classical dynamics where particle-particle interactions must be taken into account — hence for systems whose Hamilton-Jacobi equation does not separate.

Nevertheless, specific symmetries and their associated invariants exist for non-linear and explicitly time-dependent Hamiltonian systems as well. The restriction is that invariants for non-autonomous systems — apart from very exceptional cases — cannot depend on the canonical variables only. In other words, invariants for time-dependent Hamiltonian systems generally depend on time explicitly. This can be deduced from the simplest non-trivial case, given by the well-known time-dependent harmonic oscillator. In addition to its dependence on the canonical variables, this invariant depends on a time-dependent auxiliary function, which in turn follows from a differential equation, referred to in the context of our approach as the auxiliary equation.

In the general non-linear and non-autonomous case, this auxiliary equation depends on the particle coordinates. As the consequence, the auxiliary equation can only be integrated *in conjunction* with the equations of motion. From this viewpoint, the $2n$ first-order canonical equations — that determine uniquely the time evolution of the n particle system — form together with the three first-order equations of the auxiliary equation a closed coupled set of $2n+3$ first-order equations that uniquely determine the invariant I. The invariant's involved nature to depend on an auxiliary function — which in turn follows from a differential equation that depends on all particle coordinates — accounts for the fact that the invariant cannot ease the problem of integrating the system's equations of motion. Yet, the invariant provides the basis to analyze the system's dynamics *a posteriori*, hence after having solved its equations of motion.

For the particular case of isotropic quadratic Hamiltonians, the dependence of the auxiliary equation on the spatial coordinates cancels. The third-order auxiliary equation may then be analytically integrated to yield a well-known non-linear second-order equation that has been derived earlier for the time-dependent harmonic oscillator.

In the special case of autonomous systems — hence Hamiltonian systems with no explicit time-dependence — the function $\xi(t) \equiv 1$ is always a solution of the auxiliary equation. With this solution, the invariant I coincides with the invariant that is given by the system's Hamiltonian H itself. In view of this result, the familiar invariant $I = H$ just represents the particular case where the auxiliary equation possesses the special solution $\xi(t) \equiv 1$ — which is exactly given for autonomous Hamiltonian systems.

In addition to the invariant $I = H$, another non-trivial invariant for autonomous systems always exists that is associated with a solution $\xi(t) \neq$ const. of the auxiliary equation. The dependence of the invariants of a Hamiltonian system on solutions $\xi(t)$ of an auxiliary equation thus constitutes a general feature — which disappears exclusively for the particular case $\xi(t) \equiv 1$ that is associated with the invariant $I = H$ of an autonomous system.

For the case of explicitly time-dependent Hamiltonian systems, solutions of the auxiliary equation with $\xi(t) =$ const. do not exist. Therefore, the invariants for non-autonomous systems *always* depend on solutions $\xi(t)$ of the auxiliary equation. The additional complexity that arises for the invariants of non-isotropic linear and general non-linear Hamiltonian systems is that the auxiliary equation now depends on the system's spatial coordinates.

Chapter 2

Systems of charged particles in continuous description

We now switch from the discrete description of Hamiltonian n-degree-of-freedom systems to a continuous approach in the realm of statistical mechanics. Thereby, the total knowledge on the particle ensemble is reduced to a probability density function that depends *continuously* on the real space and conjugate momentum coordinates. By virtue of this description, the knowledge on the actual system state is rendered *incomplete*, inducing the phenomenon of *irreversibility* to emerge [4]. As the consequence, a modified concept for the basic equations of motion is required. In the case of particles interacting weakly through an inverse square force law, this concept is realized combining the Vlasov-Poisson equation with the Fokker-Planck equation. We shall demonstrate that this approach provides an adequate description of the particular problem of “intra-beam scattering”, occurring for charged particle beams that circulate in storage rings.

2.1 Continuous Hamiltonian systems

2.1.1 μ-phase-space Liouville theorem

We now abandon the idea of tracking the phase-space location of individual particles in favor of a global viewpoint based on a probability density that describes the particle ensemble as a whole in a continuous model. For this continuous description of a given ensemble of interacting particles, we define a 6-dimensional normalized μ-phase-space probability density function

$$f = f(\boldsymbol{x}, \boldsymbol{p}, t) \,. \tag{2.1}$$

Here, the bold symbols denote the vectors of continuous variables, namely, the three-dimensional configuration space variables $\boldsymbol{x} = (x_1, x_2, x_3)$, and $\boldsymbol{p} = (p_1, p_2, p_3)$ the corresponding vector for the conjugate momenta. The quantity $f \, d\boldsymbol{x} \, d\boldsymbol{p}$ then represents the probability of finding a particle inside a volume $d\boldsymbol{x} \, d\boldsymbol{p}$ around the phase-space point $(\boldsymbol{x}, \boldsymbol{p})$ at time t. By virtue of this definition, the probability density f constitutes a *continuous* function of its arguments. Our approach thus aims to analyze the dynamics of the probability assignment given by density function f.

The condition for no particle losses pertaining to the discrete description translates within the continuous description into the postulation of a continuity equation for the probability density $f(\boldsymbol{x}, \boldsymbol{p}, t)$. With $\boldsymbol{j} = f \cdot (\dot{\boldsymbol{x}}, \dot{\boldsymbol{p}})$ the μ-phase-space current density, the continuity equation writes

$$\frac{\partial f}{\partial t} + \operatorname{div} \boldsymbol{j} = 0 \,,$$

which means explicitly

$$\frac{\partial f}{\partial t}+\sum_{i=1}^{3}\left(\dot{x}_i\frac{\partial f}{\partial x_i}+\dot{p}_i\frac{\partial f}{\partial p_i}+f\frac{\partial \dot{x}_i}{\partial x_i}+f\frac{\partial \dot{p}_i}{\partial p_i}\right)=0\,. \tag{2.2}$$

Provided that a continuous Hamiltonian function $H:\mathbb{R}^6\times\mathbb{R}\to\mathbb{R}$, $H=H(\boldsymbol{x},\boldsymbol{p},t)$ exists that describes the system's time evolution, we can make use of the canonical equations

$$\dot{p}_i=-\frac{\partial H}{\partial x_i}\,,\qquad \dot{x}_i=\frac{\partial H}{\partial p_i}\,,\qquad i=1,2,3 \tag{2.3}$$

to eliminate the last two terms of the sum in Eq. (2.2)

$$\frac{\partial \dot{x}_i}{\partial x_i}=\frac{\partial^2 H}{\partial x_i\partial p_i}=-\frac{\partial \dot{p}_i}{\partial p_i}\,,\qquad i=1,2,3\,.$$

Equation (2.2) thus reduces to

$$\frac{\partial f}{\partial t}+\sum_{i=1}^{3}\left(\dot{x}_i\frac{\partial f}{\partial x_i}+\dot{p}_i\frac{\partial f}{\partial p_i}\right)=\frac{df}{dt}=0\,, \tag{2.4}$$

which constitutes the equation of motion for the probability density function $f=f(\boldsymbol{x},\boldsymbol{p},t)$. Equation (2.4) is commonly referred to as "Liouville's theorem", but must clearly be distinguished from the proper Liouville theorem reviewed in Sec. 1.1.3. In contrast to the general Liouville theorem that applies to dynamical systems of n degrees of freedom, the μ-phase-space Liouville theorem only holds for systems that allow for a *continuous* description of its phase-space dynamics.

2.1.2 Invariant I in the continuous description

For simplicity, we restrict ourselves at this point to cases without damping — although the formalism worked out in the preceding chapter can straightforwardly be rewritten for continuous systems that include damping. For a system described by the Hamiltonian

$$H(\boldsymbol{x},\boldsymbol{p},t)=\sum_{i=1}^{3}\frac{p_i^2}{2m}+V(\boldsymbol{x},t)\,, \tag{2.5}$$

the invariant I emerges as well as a smooth function of the μ-phase-space coordinates $\boldsymbol{x}$ and $\boldsymbol{p}$

$$I(\boldsymbol{x},\boldsymbol{p},t)=\xi(t)\,H-\tfrac{1}{2}\dot{\xi}\,\boldsymbol{x}\boldsymbol{p}+\tfrac{1}{4}m\ddot{\xi}\,\boldsymbol{x}^2\,, \tag{2.6}$$

with the function $\xi=\xi(t)$ defined as a solution of the auxiliary equation

$$\tfrac{1}{4}m\dddot{\xi}\sum_{i=1}^{3}x_i^2+\dot{\xi}\left[V(\boldsymbol{x},t)+\tfrac{1}{2}\sum_{i=1}^{3}x_i\frac{\partial V(\boldsymbol{x},t)}{\partial x_i}\right]+\xi\,\frac{\partial V(\boldsymbol{x},t)}{\partial t}=0\,. \tag{2.7}$$

Similar to the auxiliary equation (1.27) of the discrete description, in general Eq. (2.7) can only be integrated in conjunction with the canonical equations (2.3).

The proof that I indeed provides a conserved quantity may again be worked out on the basis of the total time derivative of Eq. (2.6). Inserting the canonical equations (2.3) into the expression for $dI/dt=0$, we immediately find the differential equation (2.7) for $\xi(t)$.

2.1.3 Condition for self-consistent phase-space distributions

Among all phase-space probability density functions $f = f(\boldsymbol{x}, \boldsymbol{p}, t)$ with their related invariants $I = I(\boldsymbol{x}, \boldsymbol{p}, t) =$ const., we now consider the particular density function f_0 that can be expressed as a function of I only

$$f_0 = f_0(I) \,. \tag{2.8}$$

With f_0 a function of its invariant I only, we may regard f_0 as the particular probability density that describes in an averaged sense a dynamical equilibrium state of the system. The equilibrium condition (2.8) may be written alternatively as the Poisson bracket condition

$$\big[f_0, I\big] = 0 \,, \tag{2.9}$$

as Poisson brackets $[f(I), I]$ vanish for arbitrary differentiable functions f, I of the phase-space variables. With the invariant I in the form of Eq. (2.6) and $\xi(t)$ a solution of the auxiliary equation (2.7), the equilibrium condition (2.9) reads in explicit form

$$\xi \frac{\partial f_0}{\partial t} - \tfrac{1}{2}\dot{\xi} \sum_{i=1}^{3} \left(p_i \frac{\partial f_0}{\partial p_i} - x_i \frac{\partial f_0}{\partial x_i} \right) + \tfrac{1}{2} m \ddot{\xi} \sum_{i=1}^{3} x_i \frac{\partial f_0}{\partial p_i} = 0 \,. \tag{2.10}$$

With the condition (2.10) fulfilled along both the solution of the equation of motion (2.4) and $\xi(t)$ as a solution of Eq. (2.7), the probability density $f_0(\boldsymbol{x}, \boldsymbol{p}, t)$ embodies an equilibrium distribution.

For the special case of an autonomous system ($\partial H / \partial t \equiv 0$), the *value* of the Hamiltonian H itself provides an invariant: $I \equiv H$. For this case, we have $\partial V(\boldsymbol{x}, t)/\partial t \equiv 0$, which means that $\xi(t) \equiv 1$ is a particular solution of the auxiliary equation (2.7). The equilibrium condition (2.10) then simplifies to

$$\frac{\partial f_0(\boldsymbol{x}, \boldsymbol{p}, t)}{\partial t} = 0 \,,$$

which obviously constitutes the equilibrium condition for autonomous systems.

2.1.4 Vlasov equation

For a system of Coulomb interacting particles, Liouville's theorem (2.4) only applies if effects emerging from the actual charge granularity can be neglected. Hence, for charged particle beams whose self-fields must be taken into account, Liouville's theorem for the μ-phase-space probability density f is fulfilled if and only if the self-fields can be approximated by a smooth (continuous) force field analogously to the smooth external focusing fields. With the smooth field analog of Eqs. (1.79) and (1.80), the equations of motion follow as

$$\dot{x}_i = \frac{p_i}{m} \,, \qquad \dot{p}_i = F_{\mathrm{ext},i}(\boldsymbol{x}, t) + q E_{\mathrm{sc},i}(\boldsymbol{x}, t) \,,$$

which contains the continuous electric self field $E_{\mathrm{sc},i}$ functions associated with the continuous phase-space probability function f, according to Coulomb's law

$$\boldsymbol{E}_{\mathrm{sc}}(\boldsymbol{x}, t) = \frac{q}{4\pi\epsilon_0} \int f(\boldsymbol{x}', \boldsymbol{p}, t) \frac{\boldsymbol{x} - \boldsymbol{x}'}{|\boldsymbol{x} - \boldsymbol{x}'|^3} d\boldsymbol{x}' d\boldsymbol{p} \,. \tag{2.11}$$

Equation (2.4) thus leads to

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} \frac{p_i}{m} \frac{\partial f}{\partial x_i} + \sum_{i=1}^{3} \Big[F_{\mathrm{ext},i}(\boldsymbol{x}, t) + q E_{\mathrm{sc},i}(\boldsymbol{x}, t) \Big] \frac{\partial f}{\partial p_i} = 0 \,, \tag{2.12}$$

which is commonly referred to as the Vlasov equation. Together with Eq. (2.11), it constitutes a closed set equations that determine uniquely the time evolution of the μ-phase-space density function f under the influence of external forces $\boldsymbol{F}_{\mathrm{ext}}(\boldsymbol{x}, t)$ and the smooth part $q\boldsymbol{E}_{\mathrm{sc},i}(\boldsymbol{x}, t)$ of the electric self-forces.

2.2 Modeling charge granularity effects with the Fokker-Planck equation

2.2.1 Langevin equation

Describing the time evolution of a system of Coulomb interacting particles on the basis of the Vlasov equation (2.12) means to exclude all effects that originate in the actual charge granularity of the "real" system. This approach may be considered appropriate for studies of beam dynamics in accelerators and beam transport sections, hence in lattices where the beam life time between source and target is short. On the other hand, charge granularity effects can no longer be neglected for the long term beam behavior in storage rings. In these structures, the effect of multiple small-angle Coulomb scattering between the beam particles — the so-called "intra-beam scattering" effects — limits the beam life times. So far, these effects can be described only on the basis the equation of motion (1.81) of Sec. 1.4.3, with

$$\big\{\boldsymbol{x}_1(t_0), \boldsymbol{p}_1(t_0), \ldots, \boldsymbol{x}_N(t_0), \boldsymbol{p}_N(t_0)\big\} \tag{2.13}$$

the initial condition for a beam consisting of a total of N particles of the same species. Equation (2.13) contains the complete information on the state of the system at time t_0. Together with the equations of motion (1.81), Eq. (2.13) defines a "reversible" system. This system is completely determined and does not contain any sources for loss of information, hence can be transformed any time span forwards as well as backwards. In principle, all effects occurring in charged particle beams can be derived from the time integration of Eq. (1.81).

Nevertheless, this picture is not adequate for the description of real N-body systems if N is very large. First of all, the requirement for the initial state (2.13) to be precisely known can never be fulfilled. In addition, the detailed knowledge of the state of all N particles is not necessary in order to determine the global beam properties we are usually interested in. Therefore, a statistical description of the time evolution of the particle ensemble is appropriate. This description must be consistent with exact solutions of Eq. (1.81) for a large number of particles N.

On the single-particle level, a statistical description means to replace the exact, fine-grained Coulomb force contained in Eq. (1.81) by its smoothed coarse-grained average force. The fine-grained aspect of the particle motion is then modeled by an additional fluctuating force $\boldsymbol{F}_{\mathrm{L}}$ that does not depend on the instantaneous particle position in real space. As pointed out by Jowett [27], this concept constitutes "an attempt to describe the effects of the neglected microscopic degrees of freedom". In order not to introduce a systematic error into the statistical description of the N-particle ensemble, this force must vanish on the ensemble average:

$$\langle \boldsymbol{F}_{\mathrm{L}} \rangle = 0\,.$$

In this statistical description, we must not conceive $\boldsymbol{F}_{\mathrm{L}}(\boldsymbol{p}, t)$ as an ordinary vector function but as a quantity that has only statistically defined properties. Fluctuating forces of this nature are usually referred to as "Langevin forces" [28].

In performing the transition from an "exact" fine-grained description of the particle ensemble according to Eq. (1.81) to a statistical description, not only the fluctuating Langevin force $\boldsymbol{F}_{\mathrm{L}}(\boldsymbol{p}, t)$ but also a force referred to as the "dynamical friction" force $\boldsymbol{F}_{\mathrm{fr}}(\boldsymbol{p}, t)$ must be introduced. For repelling forces, the mechanism of dynamical friction is sketched in Fig. 2.1. We observe that the deceleration of the leftmost particle in the horizontal direction before its closest encounter with the other particles is greater than its acceleration afterwards. This means that a net deceleration, hence a friction occurs. As is easily verified, the same is true for attracting forces.

In the statistical description, the N-particle ensemble is described in terms of a smooth probability density $f(\boldsymbol{x}, \boldsymbol{p}, t)$. Accordingly, the self-field appears now as a smooth function of $\boldsymbol{x}$ and t

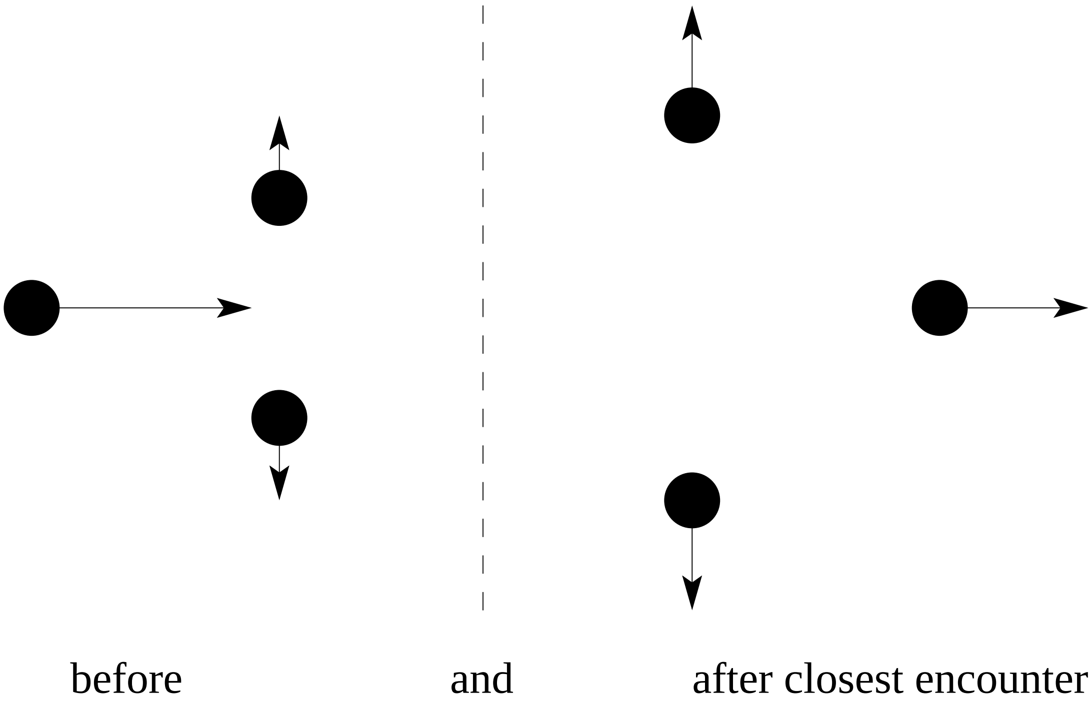

Figure 2.1: Sketch of the mechanism of dynamical friction for repelling forces between particles.

that is equivalent to a smooth external force field. The stochastic counterpart of the deterministic single-particle equation of motion (1.81) can now be written as

$$m\frac{d^2}{dt^2}\boldsymbol{x} = \boldsymbol{F}_{\text{ext}} + q\boldsymbol{E}_{\text{sc}} + \boldsymbol{F}_{\text{fr}} + \boldsymbol{F}_{\text{L}}\,, \tag{2.14}$$

containing the smooth part of the Coulomb force $\boldsymbol{E}_{\text{sc}}(\boldsymbol{x}, t)$, the dynamical friction force $\boldsymbol{F}_{\text{fr}}(\boldsymbol{p}, t)$, and the fluctuating Langevin force $\boldsymbol{F}_{\text{L}}(\boldsymbol{p}, t)$. As usual, we assumed that stochastic effects in our description are independent of the "external" force functions $\boldsymbol{F}_{\text{ext}}(\boldsymbol{x}, t)$ and $q\boldsymbol{E}_{\text{sc}}(\boldsymbol{x}, t)$. This means that the Langevin force $\boldsymbol{F}_{\text{L}}$ as well as the friction force $\boldsymbol{F}_{\text{fr}}$ do not depend on the position $\boldsymbol{x}$ in real space.

Each individual particle encounters a specific realization of the Langevin force $\boldsymbol{F}_{\text{L}}(\boldsymbol{p}, t)$. As these forces are defined by their statistical properties only, a direct integration of Eq. (2.14) is not possible. On the other hand, a deterministic equation of motion for the phase-space probability density $f(\boldsymbol{x}, \boldsymbol{p}, t)$ can be derived on the basis of Eq. (2.14). This topic will be reviewed in the following section.

2.2.2 Fokker-Planck Equation

We define $\boldsymbol{q} \equiv (\boldsymbol{x}, \boldsymbol{p})$ as the position vector in the 6-dimensional μ-phase space. If the function $f(\boldsymbol{q}, t)$ represents a normalized phase-space probability density, then $f\,d\boldsymbol{q}$ provides the probability of finding a particle inside a volume $d\boldsymbol{q}$ around the phase-space point $\boldsymbol{q}$ at time t. In these terms, the generalization of Eq. (2.14) can be written as

$$\dot{q}_i = K_i(\boldsymbol{q}, t) + \Gamma_i(\boldsymbol{q}, t)\,, \qquad i = 1, \ldots, 6\,, \tag{2.15}$$

with smooth functions $K_i(\boldsymbol{q}, t)$ and the random variables $\Gamma_i(\boldsymbol{q}, t)$ that vanish on the ensemble average. We now assume the random variables $\Gamma_i(\boldsymbol{q}, t)$ to be Gaussian-distributed and their time correlation to be given by the δ-function

$$\left\langle \Gamma_i(\boldsymbol{q},t)\,\Gamma_j(\boldsymbol{q},t')\right\rangle = 2Q_{ij}(\boldsymbol{q},t)\,\delta(t-t')\,. \tag{2.16}$$

Under these conditions, the Kramers-Moyal expansion for $\partial f(\boldsymbol{q},t)/\partial t$ terminates after the second term [29, 30, 31]. The expansion with only the first and second terms is usually called the Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \boldsymbol{L} f\,, \tag{2.17}$$

with the Fokker-Planck operator $\boldsymbol{L}$ given by

$$\boldsymbol{L} = -\sum_{i=1}^{6}\frac{\partial}{\partial q_i}K_i(\boldsymbol{q},t) + \sum_{i=1}^{6}\sum_{j=1}^{6}\frac{\partial^2}{\partial q_i\partial q_j}Q_{ij}(\boldsymbol{q},t)\,. \tag{2.18}$$

We observe that $\boldsymbol{L}$ contains quantities with non-statistical properties only: the coefficients Q_{ij} are determined by the amplitude of the δ-correlated noise functions Γ_i according to Eq. (2.16), whereas the K_i are defined by Eq. (2.15). Consequently, Eq. (2.17) represents the *deterministic* equation of motion for the probability density $f(\boldsymbol{q},t)$. It is uniquely determined by the coupled set of Langevin equations (2.15) provided that Eq. (2.16) holds.

In terms of the special Langevin equation (2.14), the Fokker-Planck operator (2.18) reduces to

$$\boldsymbol{L} = \sum_{i=1}^{3}\left[-\frac{1}{m}\frac{\partial}{\partial x_i}p_i - \frac{\partial}{\partial p_i}F_{\text{tot},i} + \frac{\partial^2}{\partial p_i^2}D_{ii}\right]\,, \tag{2.19}$$

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

$$F_{\text{tot},i}(\boldsymbol{x},\boldsymbol{p},t) = F_{\text{ext},i}(\boldsymbol{x},t) + qE_{\text{sc},i}(\boldsymbol{x},t) + F_{\text{fr},i}(\boldsymbol{p},t)\,,$$

and the momentum diffusion coefficients, measured in momentum squared per time

$$\left\langle F_{\text{L},i}(p_i,t)\;F_{\text{L},j}(p_j,t')\right\rangle = 2D_{ii}(p_i,t)\delta_{ij}\,\delta(t-t')\,. \tag{2.20}$$

In standard SI units, D_{ii} is determined by $\dim D_{ii} = \text{kg}^2\text{m}^2\text{s}^{-3}$. The off-diagonal terms of the diffusion matrix D_{ij} vanish since the Langevin forces in Eq. (2.14) are not correlated for different degrees of freedom. Correspondingly, the friction forces $F_{\text{fr},i}$ depend on p_i only. From the visualization of dynamical friction, sketched in Fig. 2.1, it is evident that these forces must always be decelerating. This means that $F_{\text{fr},i}$ changes sign as p_i does; hence, it must be an odd function of p_i. With regard to Eq. (2.20), the momentum diffusion coefficients of Eq. (2.19) turn out to be even functions of the p_i

$$F_{\text{fr},i}(p_i) = -F_{\text{fr},i}(-p_i)\,,\qquad D_{ii}(p_i) = D_{ii}(-p_i)\,. \tag{2.21}$$

A Fokker-Planck equation that describes the evolution of the probability density f associated with the stochastic motion of particles in external force fields is often referred to as Kramers' equation. As will be shown in the Sec. 2.2.4, where we investigate equilibrium solutions of Eq. (2.17), the diffusion coefficients $D_{ii}(p_i,t)$ are uniquely determined by the friction forces $F_{\text{fr},i}(p_i,t)$.

2.2.3 Fokker-Planck coefficients under time reversal

In order to show that the Fokker-Planck equation (2.17) indeed describes the emerging of irreversibility, we perform a transformation that reverses the direction of time flow [3]

$$t \to -t\,,\qquad x_i \to x_i\,,\qquad p_i \to -p_i\,.$$

Obviously, the positions x_i and hence all quantities that only depend on the positions do not change sign under this transformation. In contrast, the momenta p_i do change sign, which means that all quantities depending on the p_i may change sign under time reversal. We may thus separate the components of the Fokker-Planck operator (2.19) with respect to their behavior under time reversal

$$\boldsymbol{L} = \boldsymbol{L}_{\text{rev}} + \boldsymbol{L}_{\text{ir}} \,.$$

The “reversible” operator $\boldsymbol{L}_{\text{rev}}$ is defined to consist of those components of Eq. (2.19) that change sign under time reversal

$$\boldsymbol{L}_{\text{rev}} = \sum_{i=1}^{3} \left[-\frac{1}{m}\frac{\partial}{\partial x_i} p_i - \frac{\partial}{\partial p_i} \left(F_{\text{ext},i} + qE_{\text{sc},i} \right) \right] \,. \tag{2.22}$$

The smooth self-field $\boldsymbol{E}_{\text{sc}}$ is obtained inserting the real-space projection of the probability density $f(\boldsymbol{x}, \boldsymbol{p}, t)$ into Poisson's equation.

The components that do not change sign constitute $\boldsymbol{L}_{\text{ir}}$,

$$\boldsymbol{L}_{\text{ir}} = \sum_{i=1}^{3} \frac{\partial}{\partial p_i} \left[-F_{\text{fr},i}(p_i, t) + \frac{\partial}{\partial p_i} D_{ii}(p_i, t) \right] \,. \tag{2.23}$$

Here we made use of Eq. (2.21), which states that under time reversal $F_{\text{fr},i}$ changes sign, whereas D_{ii} does not change sign. The external forces $F_{\text{ext},i}$ have been assumed to be not velocity dependent.

Since $\partial f/\partial t$ changes sign on time reversal, a Fokker-Planck equation with only $\boldsymbol{L}_{\text{rev}}$ remains unchanged if the direction of time flow is reversed. It therefore describes the reversible transformation of the probability density function $f(\boldsymbol{x}, \boldsymbol{p}, t)$. This means that earlier states are fully restored if a reversed time integration of Eq. (2.17) is carried out with $\boldsymbol{L} \equiv \boldsymbol{L}_{\text{rev}}$ — just like a movie that is reversed at some instant of time t_0. Correspondingly, $\boldsymbol{L}_{\text{ir}}$ describes exactly those effects that do *not* depend on the direction of time flow. In other words, it describes the irreversible aspects of the system's time evolution. With $\boldsymbol{L}_{\text{ir}} = 0$, Eq. (2.17) is commonly referred to as the Vlasov equation.

2.2.4 Equilibrium distributions in autonomous systems

If the external force $\boldsymbol{F}_{\text{ext}}(\boldsymbol{x})$ contained in Eq. (2.19) is not explicitly time dependent, a stationary solution $\boldsymbol{L} f_{\text{st}} = 0$ may exist. If it exists, it can equivalently be written in terms of a function ϕ_{st} as

$$f_{\text{st}}(\boldsymbol{x}, \boldsymbol{p}) = g_0^{-1} \exp\left\{ -\phi_{\text{st}}(\boldsymbol{x}, \boldsymbol{p}) \right\} \,, \tag{2.24}$$

with $g_0 = \int \exp\left\{-\phi_{\text{st}}(\boldsymbol{x}, \boldsymbol{p})\right\} d\boldsymbol{x} d\boldsymbol{p}$ the normalization factor. We may define the irreversible probability current $S_{p_i}^{\text{ir}}$ flowing in the p_i-direction in phase space by

$$\boldsymbol{L}_{\text{ir},i} f = -\frac{\partial}{\partial p_i} S_{p_i}^{\text{ir}} \,.$$

Evidently, all irreversible currents $S_{p_i}^{\text{ir}}$ must vanish for $f = f_{\text{st}}$ to be stationary. With $\boldsymbol{L}_{\text{ir},i}$ given by Eq. (2.23), this means, explicitly,

$$F_{\text{fr},i}(p_i) = \frac{\partial D_{ii}(p_i)}{\partial p_i} - D_{ii}(p_i) \frac{\partial \phi_{\text{st}}(\boldsymbol{x}, \boldsymbol{p})}{\partial p_i} \,. \tag{2.25}$$

Equation (2.25) states that for a given ϕ_{st}, the diffusion function $D_{ii}(p_i)$ is uniquely determined by the friction force function $F_{\text{fr},i}$ — and vice versa. This mutual dependency of the diffusion effects — driving a system away from its steady state — and damping effects that cause the decay of these deviations constitutes the physical content of “fluctuation-dissipation theorems”.

In agreement with Eq. (2.21), we express the friction force function $F_{\mathrm{fr},i}$ and the momentum diffusion function D_{ii} as odd and even power series in p_i, respectively,

$$F_{\mathrm{fr},i}(p_i) = -\sum_{k=0}^{\infty} a_k\, p_i^{2k+1}\,, \qquad D_{ii}(p_i) = \sum_{k=0}^{\infty} b_k\, p_i^{2k}\,. \tag{2.26}$$

Here we assumed the coefficients a_k, b_k not to depend on $\boldsymbol{x}$ — in accordance with the precondition that the stochastic forces are not affected by the external forces. Furthermore, the coefficients a_k and b_k do not depend on the degree of freedom i by virtue of the power series (2.26). This simplification appears justified as long as the mechanism giving rise to dynamical friction can be regarded isotropic.

Inserting the power series (2.26) into Eq. (2.25), we find that $\partial\phi_{\mathrm{st}}/\partial p_i$ must be a linear function of p_i that does not depend on $\boldsymbol{x}$. Therefore, ϕ_{st} may always be separated as

$$\phi_{\mathrm{st}}(\boldsymbol{x},\boldsymbol{p}) = \psi_{\mathrm{st}}(\boldsymbol{x}) + \sum_{i=1}^{3} \frac{p_i^2}{2\left\langle p_i^2\right\rangle}\,, \tag{2.27}$$

the angle brackets denoting the respective averages over the phase-space density function: $\langle a\rangle = \int a f d\boldsymbol{x} d\boldsymbol{v}$. The quantity $\left\langle p_i^2\right\rangle$ thus embodies the second moment of the momentum p_i for the equilibrium distribution f_{st}. In a state of equilibrium these moments must agree for all degrees of freedom. Then, we may relate $\left\langle p_i^2\right\rangle$ to the equilibrium temperature T_{eq} according to

$$mk_B T_{\mathrm{eq}} = \left\langle p_i^2\right\rangle\,, \qquad i = 1,2,3\,, \tag{2.28}$$

with k_B denoting Boltzmann’s constant.

Inserting Eq. (2.27) into the Fokker-Planck equation (2.17), (2.19), the generalized potential $\psi_{\mathrm{st}}(\boldsymbol{x})$ follows from

$$\nabla\psi_{\mathrm{st}}(\boldsymbol{x}) = -\frac{1}{k_B T_{\mathrm{eq}}}\left(\boldsymbol{F}_{\mathrm{ext}}(\boldsymbol{x}) + q\boldsymbol{E}_{\mathrm{sc}}(\boldsymbol{x})\right)\,.$$

In final form, the equilibrium probability density of the Fokker-Planck equation (2.17) reads

$$f_{\mathrm{st}}(\boldsymbol{x},\boldsymbol{p}) = g_0^{-1}\exp\left\{-\psi_{\mathrm{st}}(\boldsymbol{x})\right\}\times\exp\left\{-\sum_{i=1}^{3}\frac{p_i^2}{2mkT_{\mathrm{eq}}}\right\}\,. \tag{2.29}$$

We summarize that the equilibrium distribution (2.29) follows directly from the assumption that the stochastic component of the particle motion is caused by isotropic Gaussian-distributed Langevin forces with a time correlation function proportional to the δ-function. For a given temperature T_{eq}, the spatial probability function following from ψ_{st} is uniquely determined by the external force $\boldsymbol{F}_{\mathrm{ext}}$, and the stationary self-field $\boldsymbol{E}_{\mathrm{sc}}$. Together with the unique velocity distribution, the entire phase-space probability density function is uniquely determined, which means that no other equilibrium distribution of Eq. (2.17) exists — in contrast to Vlasov systems where friction, as well as diffusion effects, vanish. If the external force function $F_{\mathrm{ext}}(\boldsymbol{x})$ does allow for an equilibrium, and if the friction is not negligible, arbitrary non-equilibrium density functions always settle down to a unique equilibrium. This is what we observe in long-term simulations of charged particle beams [32, 33]. Regardless of our initial phase-space filling, we always end up with a Gaussian velocity distribution if no resonance effects are involved.

2.3 Entropy concept

2.3.1 Definition of the μ-phase-space entropy

Following Boltzmann [3, 34], we define the entropy S pertaining to a μ-phase-space probability density function (2.1) as

$$S(t) = -k_B \int f \,\ln f \, d\boldsymbol{x} d\boldsymbol{p} \,. \tag{2.30}$$

The entropy change, hence the time derivative of Eq. (2.30), then follows as

$$\frac{dS}{dt} = -k_B \int (1 + \ln f) \, \frac{\partial f}{\partial t} \, d\boldsymbol{x} d\boldsymbol{p} \,. \tag{2.31}$$

Complying with our continuous description of particle dynamics that is based on a probability density $f(\boldsymbol{x}, \boldsymbol{p}, t)$, this entropy definition applies for the limit of an *infinite* resolution.

2.3.2 Entropy conservation for Vlasov dynamics

Under the condition that the μ-phase-space Liouville theorem applies, we can insert $\partial f / \partial t$ of Eq. (2.4) into (2.31)

$$\frac{1}{k_B} \frac{dS}{dt} = \int (1 + \ln f) \sum_{i=1}^{3} \left(\dot{x}_i \frac{\partial f}{\partial x_i} + \dot{p}_i \frac{\partial f}{\partial p_i} \right) \, d\boldsymbol{x} d\boldsymbol{p} \,.$$

Integration by parts over all phase space yields

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

if we make the reasonable physical assumption that the phase-space density f as well as all its derivatives vanish at the boundaries of the populated phase space. Then, all integrated expressions evaluate to zero at the integration boundaries. Summarizing the above result, we may state that Liouville's theorem implies the conservation of the infinite resolution entropy (2.30)

$$\frac{df}{dt} = 0 \quad \Longrightarrow \quad \frac{dS}{dt} = 0 \,. \tag{2.32}$$

As has been discussed in Sec. 2.2, Liouville's theorem for the μ-phase space does not apply if the system's dynamics comprises non-negligible interactions between individual particles. According to (2.32), entropy changes are related to violations of the μ-phase-space Liouville theorem. Processes that cause a phase-space filamentation while *conserving* the μ-phase-space Liouville theorem do *not* change the entropy S, as defined in Eq. (2.30). In the case of charged particle beams, such a phase-space filamentation means a loss of beam quality in a practical sense due to a lack of means to reestablish the original phase-space state. Yet our definition of entropy S does not reflected such processes since, in the infinite resolution limit, a filamentation does not mean a loss of beam quality.

2.3.3 Entropy change associated with a non-Liouvillean process

As we have seen in the previous section, the change of entropy (2.31) vanishes as log as the time evolution of the probability density f follows from Vlasov's equation (2.4). Therefore, only the irreversible part $\boldsymbol{L}_{\text{ir}}$ of the Fokker-Planck operator $\boldsymbol{L}$, as given by Eq. (2.23), may contribute to a change of entropy S

$$\left[\frac{\partial f}{\partial t} \right]_{\text{ir}} = \boldsymbol{L}_{\text{ir}} f \,. \tag{2.33}$$

Equation (2.31) thus writes, explicitly

$$\frac{1}{k_B}\frac{dS}{dt} = \int (1+\ln f)\left\{ \sum_i \frac{\partial}{\partial p_i}\left[F_{\mathrm{fr},i}(\boldsymbol{p},t)\,f\right] - \sum_i\sum_j \frac{\partial^2}{\partial p_i \partial p_j}\left[D_{ij}(\boldsymbol{p},t)\,f\right]\right\} d\boldsymbol{x}d\boldsymbol{p}\,. \quad (2.34)$$

Integrating the terms of the first sum twice by parts, we obtain

$$\int (1+\ln f)\,\frac{\partial}{\partial p_i}\big[F_{\mathrm{fr},i} f\big]\, d\boldsymbol{x}d\boldsymbol{p} = \int \frac{\partial F_{\mathrm{fr},i}}{\partial p_i} f\, d\boldsymbol{x}d\boldsymbol{p}\,.$$

Again, we assume that all derivatives of f vanish at the boundary of the populated phase space.

To integrate the second sum of Eq. (2.34), the phase-space density function f must be given. This will be worked out here on the basis of of a non-isotropic Maxwell-Boltzmann distribution that generalizes the steady state idealization of Eq. (2.29)

$$f(\boldsymbol{x},\boldsymbol{p},t) = g(\boldsymbol{x},t)\times\exp\left\{-\sum_{i=1}^{3}\frac{p_i^2}{2mk_BT_i}\right\}\,. \quad (2.35)$$

Herein, $g(\boldsymbol{x},t)$ denotes the self-consistent charge density. The "non-equilibrium temperature" T_i pertaining to the i-th degree of freedom that is contained in the exponential function of Eq. (2.35) describes the incoherent part of the kinetic particle energy

$$mk_BT_i = \left\langle \left(p_i^{\mathrm{inc}}\right)^2\right\rangle\,.$$

We will address the notation of "non-equilibrium temperatures" in more detail in Sec. 2.4.2.

With the phase-space density function (2.35), the terms of the second sum of Eq. (2.34) evaluate to

$$\int (1+\ln f)\,\frac{\partial^2}{\partial p_i \partial p_j}\big[D_{ij} f\big]\, d\boldsymbol{x}d\boldsymbol{p} = -\frac{\delta_{ij}}{mk_BT_i}\int D_{ij} f\, d\boldsymbol{x}d\boldsymbol{p}\,.$$

Finally, the change of entropy caused by a non-vanishing Fokker-Planck operator $\boldsymbol{L}_{\mathrm{ir}}$ can be expressed in terms of the Fokker-Planck coefficients as

$$\frac{1}{k_B}\frac{dS}{dt} = \sum_{i=1}^{3}\left(\left\langle\frac{\partial F_{\mathrm{fr},i}}{\partial p_i}\right\rangle + \frac{\langle D_{ii}\rangle}{mk_BT_i}\right)\,, \quad (2.36)$$

with the angle brackets denote again the respective averages over the μ-phase-space density function f.

2.3.4 Ornstein-Uhlenbeck processes

The Fokker-Planck model — as expressed mathematically in Eq. (2.33) — is based on the assumption that the action of the stochastic components of the interaction forces can be described in terms of a diffusion process in momentum space that is opposed by a dynamical friction force. If these stochastic contributions to the dynamics of a system are small, we may restrict ourselves to a subset of Markov processes, referred to as Ornstein-Uhlenbeck processes [35]. The latter are defined by the property that the underlying Fokker-Planck equation contains a linear drift coefficient together with a constant diffusion coefficient

$$F_{\mathrm{fr},i} = -\beta_{\mathrm{fr},i}\,p_i\,, \qquad \beta_{\mathrm{fr},i},\ D_{ii} = \text{const.} \quad (2.37)$$

This Ansatz corresponds to Stokes's friction law in classical mechanics. It applies to cases where the friction forces are small in comparison to all other forces relevant for the dynamics of the system. This is true in our context, since taking into account friction effects among the beam particles always plays the role of a small correction. With Eq. (2.37), the relation for the entropy change (2.36) of Ornstein-Uhlenbeck processes follows as

$$\frac{1}{k_B}\frac{dS}{dt} = \sum_{i=1}^{3}\left(-\beta_{\mathrm{fr},i} + \frac{D_{ii}}{mk_BT_i}\right) . \tag{2.38}$$

Equation (2.38) forms the basis for establishing a relation between entropy and rms emittance, as will be shown in Sec 2.4.3.

At this point it is interesting to consider the special case of isotropic Fokker-Planck coefficients. This is surely correct for situations not too far from a fictitious thermodynamic equilibrium where the diffusion as well as the friction processes can be treated as approximately isotropic. Equation (2.38) then becomes

$$\frac{1}{k_B}\frac{dS}{dt} = \sum_{i=1}^{3}\left(-\beta_{\mathrm{fr}} + \frac{D}{mk_BT_i}\right) .$$

The diffusion process arising from the fluctuations of the self-fields and the friction effects associated with particle-particle interactions are *not* independent of each other. On the contrary, the momentum diffusion coefficients D_{ii} are related to the friction terms $\beta_{\mathrm{fr},i}$ via a fluctuation-dissipation theorem. In the simplest case of an isotropic process, this theorem is embodied in the Einstein relation [36]

$$D = \beta_{\mathrm{fr}}\, mk_BT_{\mathrm{eq}} . \tag{2.39}$$

Herein, T_{eq} stands for the temperature of the equilibrium state. We must recall here that "temperature" denotes the incoherent part of the system's kinetic energy. For a system with "non-equilibrium temperatures" that is oscillating anisotropicly around T_{eq}, the equilibrium temperature can therefore be approximated by the arithmetic average of the T_i

$$T_{\mathrm{eq}} = \tfrac{1}{3}\sum_{i=1}^{3} T_i .$$

The entropy change due to a temperature balancing process may then be written as

$$\frac{1}{k_B}\frac{dS}{dt} = \beta_{\mathrm{fr}}\sum_{i=1}^{3}\left(\frac{T_{\mathrm{eq}}}{T_i} - 1\right) , \tag{2.40}$$

or, explicitly

$$\frac{1}{k_B}\frac{dS}{dt} = \tfrac{1}{3}\beta_{\mathrm{fr}}\left[\frac{(T_x-T_y)^2}{T_xT_y} + \frac{(T_x-T_z)^2}{T_xT_z} + \frac{(T_y-T_z)^2}{T_yT_z}\right] . \tag{2.41}$$

Obviously, the entropy $S(t)$ remains unchanged in the case of temperature equilibrium while increasing during temperature balancing

$$\frac{dS}{dt}\begin{cases} = 0 & \text{for temperature equilibrium,} \\ > 0 & \text{during temperature balancing.}\end{cases}$$

We may regard Eq. (2.41) as a particular manifestation of Boltzmann's H-theorem [3]. The total heat exchange dQ/dt vanishes, as is easily seen from Eq. (2.40)

$$\frac{dQ}{dt} \equiv \sum_{i=1}^{3} T_i\frac{dS_i}{dt} = k_B\beta_{\mathrm{fr}}\sum_{i=1}^{3}\big(T_{\mathrm{eq}} - T_i\big) \equiv 0 . \tag{2.42}$$

If we exclude effects such as radiation damping or dissipation of electro-magnetic energy in the surrounding structure and assume that no external heating or cooling devices are active, this vanishing of the total heat exchange is not surprising since a charged particle beam cannot exchange heat with the focusing lattice. Within the beam, heat exchange between the degrees of freedom may occur, leading to an entropy growth as described by Eq. (2.41). We conclude that equipartitioning effects occurring within thermally unbalanced charged particle beams are always associated with an irreversible degradation of the beam quality as a whole. In real focusing lattices consisting of isolated lenses that are separated by drift spaces, temperature differences always exist even if the beam is perfectly matched to the focusing period. Therefore, a certain growth rate — depending on the size of the temperature differences — can never be avoided.

This process is observed for charged particle beams in storage rings, commonly referred to as intra-beam scattering. The time scale for this process is determined by the frequency β_{fr}. The procedure to determine this quantity for intra-beam scattering effects in charged particle beam will be discussed in Sec. 2.4.5.

2.4 Solutions of the Vlasov-Fokker-Planck equation

2.4.1 Moment analysis of the Vlasov-Fokker-Planck equation

The general Fokker-Planck equation (2.17) embodies the closed equation motion for the continuous probability density f that is subject to both Hamiltonian and non-Hamiltonian forces. We have seen that the Hamiltonian part of the forces complies with Liouville's theorem (2.4) and accounts for the reversible aspects of the system's time evolution. As has been shown is Sec. 2.2.3, the non-Hamiltonian forces account for the irreversible aspects of system's dynamics. In closed form, the two parts of the equation for of motion for $f(\boldsymbol{x},\boldsymbol{p},t)$ writes

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} \left[\frac{p_i}{m} \frac{\partial f}{\partial x_i} + \Big(F_{\text{ext},i} + qE_{\text{sc},i} \Big) \frac{\partial f}{\partial p_i} \right] = \left[\frac{\partial f}{\partial t} \right]_{\text{ir}} , \tag{2.43}$$

with the equation for the irreversible effects given by

$$\left[\frac{\partial f}{\partial t} \right]_{\text{ir}} = -\sum_{i=1}^{3} \frac{\partial}{\partial p_i} \left[F_{\text{fr},i}(\boldsymbol{p},t)\, f \right] + \sum_{i,j=1}^{3} \frac{\partial^2}{\partial p_i \partial p_j} \left[D_{ij}(\boldsymbol{p},t)\, f \right] .$$

The relation between f and the self-field $\boldsymbol{E}_{\text{sc}}$ is provided by Coulomb's law (2.11). In most cases of practical interest, a direct integration of Eq. (2.43) seems not appropriate as we are usually not interested the detailed knowledge of the phase-space probability density. A usual way to switch to more global physical quantities is to consider "second moments" [7, 8] of f, similar to

$$\left\langle x^2 \right\rangle = \int x^2\, f\, d\boldsymbol{x} d\boldsymbol{p} \,.$$

$\sqrt{\langle x^2 \rangle}$ has the physical interpretation of being proportional to the actual beam width in x. Our purpose is now to derive the equations of motion for the *moments* of f from the closed equation of motion for $f(\boldsymbol{x},\boldsymbol{p},t)$, embodied in the Vlasov-Fokker-Planck equation (2.43). As these moment equations do not comprise anymore the detailed information on the time evolution of the probability density f, we expect them to be much easier to integrate. Nevertheless, a problem arises from the fact that — in contrast to Eq. (2.43) — the moment equations are no longer closed. This means that the equations of motion for the second moments of f generally depend on higher order moments, which leads to a infinite series of coupled moment equations, commonly referred to as the "BBGKY hierarchy" [3, 37]. In order to find an approximate solution for the moment equations, hence to render the moment equations closed, we must therefore find an appropriate truncation scheme for the infinite hierarchy.

In order to set up the equation of motion for the second moments of f, we calculate the respective time derivatives according to

$$\frac{d}{dt}\left\langle x^2\right\rangle = \int x^2\,\frac{\partial f}{\partial t} d\boldsymbol{x} d\boldsymbol{p}\,,$$

with $\partial f/\partial t$ given by Eq. (2.43). In total, the second-order moment analysis of the Fokker-Planck equation (2.43) yields the following set of coupled moment equations for each phase-space plane $i = 1, 2, 3$:

$$\frac{d}{dt}\left\langle x_i^2\right\rangle - \frac{2}{m}\left\langle x_i p_i\right\rangle = 0\,, \tag{2.44a}$$

$$\frac{d}{dt}\left\langle x_i p_i\right\rangle - \frac{1}{m}\left\langle p_i^2\right\rangle - \left\langle x_i F_{\text{ext},i}\right\rangle - q\left\langle x_i E_{\text{sc},i}\right\rangle = \left\langle x_i F_{\text{fr},i}\right\rangle\,, \tag{2.44b}$$

$$\frac{d}{dt}\left\langle p_i^2\right\rangle - 2\left\langle p_i F_{\text{ext},i}\right\rangle - 2q\left\langle p_i E_{\text{sc},i}\right\rangle = 2\left\langle p_i F_{\text{fr},i}\right\rangle + 2\left\langle D_{ii}\right\rangle\,. \tag{2.44c}$$

The rms emittance ε_i pertaining to the i-th direction in the beam system is commonly defined as

$$\varepsilon_i^2(t) = \left\langle x_i^2\right\rangle\left\langle p_i^2\right\rangle - \left\langle x_i p_i\right\rangle^2. \tag{2.45}$$

With $F_{\text{fr},i}$ from Eq. (2.37), linear external focusing forces

$$F_{\text{ext},i} = -m\,\omega_i^2(t)\,x_i\,, \tag{2.46}$$

and Sacherer's [8] representation of $\left\langle x_i E_{\text{sc},i}\right\rangle$ that holds for unbunched beams with elliptic cross section in real space

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

we obtain the envelope equation from the first two moment equations (2.44)

$$\frac{d^2}{dt^2}\sqrt{\left\langle x_i^2\right\rangle} + \beta_{\text{fr},i}\frac{d}{dt}\sqrt{\left\langle x_i^2\right\rangle} + \omega_i^2(t)\sqrt{\left\langle x_i^2\right\rangle} - \frac{qI}{4\pi\epsilon_0 mc\beta}\,\frac{1}{\sqrt{\left\langle x^2\right\rangle} + \sqrt{\left\langle y^2\right\rangle}} - \frac{\varepsilon_i^2(t)/m^2}{\sqrt{\left\langle x_i^2\right\rangle}^3} = 0\,. \tag{2.47}$$

Calculating the time derivative of Eq. (2.45), and inserting the moment equations (2.44), we find that three distinct sources for the rms emittance change can be distinguished

$$\frac{d}{dt}\varepsilon_i^2(t) = \left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\text{ext}} + \left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\text{sc}} + \left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\text{ir}}\,, \tag{2.48}$$

namely, the external field contribution, the contribution related to the smooth space-charge fields, and the contribution due to the Langevin forces described by the irreversible part (2.23) of the Fokker-Planck operator.

If the external focusing forces are linear, their contribution to the change of the rms emittance vanishes

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

The contribution to the rms emittance change due to the smooth space-charge field $\boldsymbol{E}_{\mathrm{sc}}$ is given by

$$\left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\mathrm{sc}} = 2q\left[\left\langle x_i^2\right\rangle\left\langle p_i E_{\mathrm{sc},i}\right\rangle - \left\langle x_i p_i\right\rangle\left\langle x_i E_{\mathrm{sc},i}\right\rangle\right]. \tag{2.49}$$

If we write this equation for all three spatial degrees of freedom, the electric field terms together form the physical quantity of "free field energy", i.e. the difference between the *actual* charge distribution's electrostatic field energy W and the field energy W_{u} of the *uniform* charge distribution having the same rms size [38, 39, 40, 41]

$$\sum_{i=1}^{3}\frac{1}{\left\langle x_i^2\right\rangle}\left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\mathrm{sc}} + \frac{2m}{N}\frac{d}{dt}\left(W - W_{\mathrm{u}}\right) = 0\,. \tag{2.50}$$

In the short-term simulation to presented in Fig. 3.2 of Sec. 3.2.1, we demonstrate that the exchange of rms emittance and "free field energy" is indeed a reversible process.

The third contribution to the change of the rms emittance emerges from the irreversible Fokker-Planck operator, as given by Eq. (2.23)

$$\left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\mathrm{ir}} = 2\left[\left\langle x_i^2\right\rangle\left\langle p_i F_{\mathrm{fr},i}\right\rangle - \left\langle x_i p_i\right\rangle\left\langle x_i F_{\mathrm{fr},i}\right\rangle + \left\langle x_i^2\right\rangle\left\langle D_{ii}\right\rangle\right]. \tag{2.51}$$

Thus, the irreversible emittance growth depends on both the Fokker-Planck coefficients *and* the specific shape of the beam envelope functions. Inserting Stokes' friction law $F_{\mathrm{fr},i} = -\beta_{\mathrm{fr}} p_i$ of Eq. (2.37) and the fluctuation-dissipation theorem in the simple form of Eq. (2.39) into Eq. (2.51), we find

$$\frac{1}{\left\langle x_i^2\right\rangle}\left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\mathrm{ir}} = 2\beta_{\mathrm{fr}}\left(mk_B T_{\mathrm{eq}} - \frac{\varepsilon_i^2(t)}{\left\langle x_i^2\right\rangle}\right). \tag{2.52}$$

Equation (2.52) represents a simple temperature relaxation equation. Together with the envelope equation (2.47), we end up with a closed set of differential equations for $\left\langle x_i^2\right\rangle$ and $\varepsilon_i^2(t)$ if we neglect the rms emittance changes due to variations of the "free field energy", as described by Eq. (2.50).

2.4.2 Beam "temperatures"

As usual in statistical physics, we relate the temperature of a particle ensemble to its "incoherent" motion. In general, charged particle beams change their size while passing through an ion optical system. The total kinetic energy $\left\langle p_i^2\right\rangle/2m$ that follows from $f(\boldsymbol{x},\boldsymbol{p},t)$ contains a coherent part if $\left\langle x_i p_i\right\rangle \neq 0$. Therefore, the coherent part of the kinetic energy must be subtracted from the total kinetic energy in order to obtain its incoherent part. The "non-equilibrium temperature" $k_B T_i$ — defined as the incoherent part of the kinetic energy of the i-th degree of freedom — is thus given by

$$mk_B T_i \equiv \left\langle\left(p_i^{\mathrm{inc}}\right)^2\right\rangle, \qquad p_i^{\mathrm{inc}} = p_i - x_i\frac{\left\langle x_i p_i\right\rangle}{\left\langle x_i^2\right\rangle}. \tag{2.53}$$

Using the rms emittance, defined by Eq. (2.45), we can then express the "non-equilibrium temperature" $k_B T_i$ of the i-th degree of freedom as

$$mk_B T_i(t) = \frac{\varepsilon_i^2(t)}{\left\langle x_i^2\right\rangle}. \tag{2.54}$$

Apart from isolated symmetry locations, the temperatures related to the spatial directions do not agree. For a coasting beam in a strong-focusing system, we have

$$T_x > T_{\mathrm{eq}} \Longleftrightarrow T_y < T_{\mathrm{eq}}$$

and vice versa. With Eq. (2.54) and $mk_BT_z = \left\langle(\Delta p_z)^2\right\rangle$, the longitudinal temperature in the beam frame, we approximate the equilibrium temperature T_{eq} by the instantaneous average of the "non-equilibrium temperatures" k_BT_i

$$mk_BT_{\mathrm{eq}} = \tfrac{1}{3}mk_B\big(T_x + T_y + T_z\big) = \frac{1}{3}\left(\frac{\varepsilon_x^2}{\langle x^2\rangle} + \frac{\varepsilon_y^2}{\langle y^2\rangle} + \left\langle(\Delta p_z)^2\right\rangle\right). \tag{2.55}$$

Of course, Eq. (2.55) cannot provide an "exact" expression for the respective equilibrium temperature T_{eq} of a given non-equilibrium system. Nevertheless, we may use it as an approximation that holds in the presence of "noise forces". The latter render the system's "memory" of earlier states finite, which justifies the approach to use the instantaneous average temperature as the equilibrium temperature. As we shall see in Sec. 2.4.4, we get a closed equation of motion for the emittance on the basis of Eq. (2.55).

2.4.3 The relation of entropy and rms emittance changes

Disregarding emittance changes due to non-linear external forces $\boldsymbol{F}_{\mathrm{ext}}$, the equation of motion for the rms emittance (2.48) can be rewritten on the basis of Eqs. (2.49), (2.51), and (2.37) as

$$\frac{1}{\left\langle x_i^2\right\rangle}\frac{d}{dt}\varepsilon_i^2(t) = 2\left[-\beta_{\mathrm{fr},i}\frac{\varepsilon_i^2(t)}{\left\langle x_i^2\right\rangle} + D_{ii} + q\left(\langle p_iE_{\mathrm{sc},i}\rangle - \frac{\langle x_ip_i\rangle}{\left\langle x_i^2\right\rangle}\langle x_iE_{\mathrm{sc},i}\rangle\right)\right]. \tag{2.56}$$

With regard to the equation for change of entropy (2.38), the "temperature" T_i can be replaced by the corresponding beam moments, according to Eq. (2.54)

$$\frac{dS}{dt} = \sum_{i=1}^{3}\frac{dS_i}{dt} \qquad , \qquad \frac{1}{k_B}\frac{dS_i}{dt} = -\beta_{\mathrm{fr},i} + \frac{\left\langle x_i^2\right\rangle}{\varepsilon_i^2(t)}D_{ii}\,. \tag{2.57}$$

Inserting Eq. (2.57) into (2.56), we obtain an equation relating emittance, entropy and free field energy

$$\frac{1}{\left\langle x_i^2\right\rangle}\frac{d}{dt}\varepsilon_i^2(t) = \frac{2}{k_B}\frac{\varepsilon_i^2(t)}{\left\langle x_i^2\right\rangle}\frac{dS_i}{dt} + 2q\left(\langle p_iE_{\mathrm{sc},i}\rangle - \frac{\langle x_ip_i\rangle}{\left\langle x_i^2\right\rangle}\langle x_iE_{\mathrm{sc},i}\rangle\right). \tag{2.58}$$

Summation over i yields

$$\sum_{i=1}^{3}\frac{1}{\left\langle x_i^2\right\rangle}\frac{d}{dt}\varepsilon_i^2(t) + \frac{2m}{N}\frac{d}{dt}\left(W - W_{\mathrm{u}}\right) = \begin{cases} 2m\displaystyle\sum_i T_i\frac{dS_i}{dt} & \text{in general} \\ 0 & \text{for isotropic FP coefficients.}\end{cases} \tag{2.59}$$

As stated before in Eq. (2.42), the right hand side of Eq. (2.59) sums up to zero under the condition of isotropic Fokker-Planck coefficients. Equation (2.59) then constitutes the known relationship between the changes of the rms emittances and the change of the free field energy, first derived by Wangler [39, 40, 42] in a pure Vlasov approach. As we learn now, this equation even holds if Liouville's theorem in the μ-phase space does not apply as long as the non-Liouvillean effects can be approximated with isotropic Fokker-Planck coefficients.

Multiplying Eq. (2.58) with $\left\langle x_i^2\right\rangle/2\varepsilon_i^2(t)$, and solving for the entropy term leads to the equivalent form

$$\frac{1}{k_B}\frac{dS_i}{dt} = \frac{d}{dt}\ln\varepsilon_i(t) - \frac{q}{\varepsilon_i^2(t)}\Big(\left\langle x_i^2\right\rangle\langle p_iE_{\mathrm{sc},i}\rangle - \langle x_ip_i\rangle\langle x_iE_{\mathrm{sc},i}\rangle\Big). \tag{2.60}$$

Summing now Eq. (2.60) over i, the time derivative of the entropy function $S(t)$ becomes

$$\frac{1}{k_B}\frac{dS}{dt} = \frac{d}{dt}\ln\varepsilon_x(t)\varepsilon_y(t)\varepsilon_z(t) - q\sum_{i=1}^{3}\frac{\langle x_i^2\rangle}{\varepsilon_i^2(t)}\left(\langle p_i E_{\mathrm{sc},i}\rangle - \frac{\langle x_i p_i\rangle}{\langle x_i^2\rangle}\langle x_i E_{\mathrm{sc},i}\rangle\right) . \tag{2.61}$$

This equation constitutes a general relation between entropy change, the change of the rms emittances, and the temperature weighted change of the free field energy for the realm of ion optics. Equation (2.61) states that the instantaneous entropy change is determined by the change of the total rms emittance $\varepsilon_x\varepsilon_y\varepsilon_z$ minus the emittance change that originates in the (reversible) change of the "free field energy". This confirms the heuristic approach presented earlier by Lawson et al. [43], who showed the close relation between the entropy and beam emittance.

We note that Eq. (2.58) as well as Eq. (2.60) do not contain any Fokker-Planck coefficients — although they are derived on the basis of the Fokker-Planck approach (2.43). Recalling Eq. (2.56), we see that the Fokker-Planck related moments exactly agree with those appearing in Eq. (2.57) — provided that we restrict ourselves to Ornstein-Uhlenbeck processes and the global temperature definition (2.54). Under these preconditions, the insertion of Eq. (2.57) into Eq. (2.56) leads to a complete replacement of all terms containing Fokker-Planck coefficients by the function for the change of entropy. The Fokker-Planck approach is thus included in Eqs. (2.58) and (2.60) just by allowing for changes of the entropy (2.30), and *not* by eliminating entropy changes dS_i a priori, as it is done implicitly in a Vlasov approach.

2.4.4 Equations for the irreversible emittance growth

Inserting the equilibrium temperature expression (2.55) into Eq. (2.52), we finally get for the irreversible emittance growth

$$\frac{1}{\langle x^2\rangle}\frac{d}{dt}\varepsilon_x^2(t)\bigg|_{\mathrm{ir}} = -\frac{2\beta_{\mathrm{fr}}}{3}\left(\frac{2\varepsilon_x^2(t)}{\langle x^2\rangle} - \frac{\varepsilon_y^2(t)}{\langle y^2\rangle} - \left\langle(\Delta p_z)^2\right\rangle\right) . \tag{2.62}$$

With the definition of the temperature ratios

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

equation (2.62) simplifies to

$$\frac{d}{dt}\ln\varepsilon_x(t)\bigg|_{\mathrm{ir}} = \tfrac{1}{3}\beta_{\mathrm{fr}}\left(r_{xy} + r_{xz} - 2\right) .$$

Obviously, the change of the emittance $\varepsilon_x(t)$ may be positive as well as negative, depending on the actual temperature ratios. Summing over all three degrees of freedom, the change of the total emittance $\varepsilon^3 = \varepsilon_x\varepsilon_y\varepsilon_z$ is found to be positive in any case

$$\frac{d}{dt}\ln\varepsilon_x\varepsilon_y\varepsilon_z\bigg|_{\mathrm{ir}} = \tfrac{1}{3}\beta_{\mathrm{fr}}\left(\frac{(1-r_{xy})^2}{r_{xy}} + \frac{(1-r_{xz})^2}{r_{xz}} + \frac{(1-r_{yz})^2}{r_{yz}}\right) \geq 0\,. \tag{2.63}$$

We thus always find a growth of ε if the coefficients of the irreversible part of the Fokker-Planck operator (2.23) do not vanish. This suggests relating the growth of ε due to non-vanishing friction and diffusion effects to a growth of the beam entropy [44, 45].

To obtain the e-folding time τ_{ef} of the total emittance $\varepsilon = \sqrt[3]{\varepsilon_x\varepsilon_y\varepsilon_z}$, we integrate Eq. (2.63) along one focusing period T

$$\tau_{\mathrm{ef}}^{-1} = \tfrac{1}{9}\,\beta_{\mathrm{fr}}\left(I_{xy} + I_{xz} + I_{yz}\right) . \tag{2.64}$$

Here, I_{xy}, I_{xz}, and I_{yz} denote the "temperature imbalance integrals" similar to

$$I_{xy} = \frac{1}{T} \int_0^T \frac{\left[1 - r_{xy}(t)\right]^2}{r_{xy}(t)} \, dt \qquad , \qquad r_{xy}(t) = \frac{\varepsilon_y^2}{\langle y^2 \rangle} \frac{\langle x^2 \rangle}{\varepsilon_x^2} \, . \tag{2.65}$$

Equation (2.62) shows that the time evolution of the emittances depends on the detailed shape of the beam widths. Therefore, the differential equations describing the growth of $\varepsilon(t)$ can be integrated only in conjunction with the envelope equations, as given for the x-direction by Eq. (2.47).

2.4.5 Fokker-Planck coefficients for intra-beam scattering

The Fokker-Planck equation (2.17) with the operator (2.19) has been derived on the basis of the stochastic differential equation (2.14). Accordingly, the coefficients $F_{\mathrm{fr},i}$ and D_{ii} contained in (2.19) are related to the dynamical friction $\boldsymbol{F}_{\mathrm{fr}}$ and the Langevin force terms $\boldsymbol{F}_{\mathrm{L}}$ of Eq. (2.14) — which in turn models the set of single-particle equations (1.81). In order to learn how the Fokker-Planck coefficients for the effect of intra-beam scattering are correlated to the physical properties of the charged particle ensemble in question, it is necessary to return to the single-particle equation (1.81), and to analyze the process of small-angle Coulomb scattering of a pair of charged particles. This has been worked out earlier by Chandrasekhar [6] and Jansen [9].

The method of evaluating the Fokker-Planck coefficients for intra-beam scattering effects within a charged particle beam can be summarized as follows:

- In the first step, the velocity changes of a test particle due to scattering from a single beam particle as a function of the test particle's initial velocity and impact parameter are calculated,
- secondly, the expression obtained in the first step is averaged over all possible impact parameters,
- finally, averaging over the particles' momentum distribution is performed. This means that the momentum distribution of the beam must be known.

Here, we assume the *equilibrium* momentum distribution to be Maxwellian. The Fokker-Planck approach provides a refinement of our description of beam dynamics that applies if the non-Liouvillean effects are small compared to the macroscopic Liouvillean forces $\boldsymbol{F}_{\mathrm{ext}}$ and $q\boldsymbol{E}_{\mathrm{sc}}$. Therefore, as the first approximation, we may assume the friction as well as the diffusion processes to be isotropic. Then only one diffusion coefficient D in conjunction with a single friction coefficient β_{fr} appears in our equations.

For the effect of intra-beam scattering, $F_{\mathrm{fr},i}$ is then obtained as [9, 32]

$$F_{\mathrm{fr},i} = -\beta_{\mathrm{fr}} \, p_i \, , \qquad \beta_{\mathrm{fr}} = \frac{16\sqrt{\pi}}{3} \left(\frac{Z^2 r_c}{A} \right)^2 n \, c \left(\frac{2k_B T_{\mathrm{eq}}}{mc^2} \right)^{-3/2} \ln \Lambda \, , \tag{2.66}$$

with $r_c = e_0^2/(4\pi\epsilon_0 mc^2)$ the classical particle radius for protons, n the particle density, T_{eq} the equilibrium temperature Eq. (2.28), and $\ln \Lambda$ the Coulomb logarithm. Of course, the assumption of isotropic diffusion and friction — embodied in a single friction coefficient β_{fr} — could be dropped. On the other hand, this would lead to more complicated equations for the temperature relaxation processes, to be presented in the following section.

2.4.6 Coupled set of envelope and temperature relaxation equations for unbunched ("coasting") beams in storage rings

We now set up the coupled system of envelope and temperature relaxation equations [46], as has been derived in Eqs. (2.47) and (2.62). For practical purposes, a translation of these equations into the laboratory system necessary. In this context, we must discuss some issues of beam dynamics in curved system in order to apply our formalism to the description of intra-beam scattering effects in storage rings.

“Trace-space” notation

For numerical calculations of given lattices, it is more convenient to use the longitudinal path length s instead of the time t as the independent variable. This can be seen if we bring to mind that each particular lattice consists of a sequence of focusing devices. Of course, the lengths of these devices are the same for all particles due to their non-relativistic relative velocities — whereas the times to cover these lengths differ.

In conjunction, we switch to the “trace-space” [37] notation for the transverse coordinates. This means that the transverse particle momenta p_x and p_y are replaced by the angles x' and y' the particle encounters with respect to the reference trajectory, as seen in the laboratory system. The respective laboratory frame quantities are marked with the subscript ℓ. With γ the relativistic mass factor, the transformation relations for the particle momenta and time t are given by

$$\begin{aligned} p_x &= mc\beta\gamma\, x'_\ell\,, \\ p_y &= mc\beta\gamma\, y'_\ell\,, \\ s &= c\beta\gamma\, t\,. \end{aligned}$$

The lattice functions $k_i(s) = \omega_i(t)/c\beta\gamma$ describe the linear external focusing forces (2.46) in the laboratory frame. Correspondingly, the transverse trace-space emittances $\bar{\varepsilon}_i$ in this frame are given by

$$\bar{\varepsilon}_i^2 = \left\langle x_i^2 \right\rangle \left\langle x_i'^2 \right\rangle - \left\langle x_i x_i' \right\rangle^2 \,, \tag{2.67}$$

which are related to the emittances (2.45) in beam system through $\bar{\varepsilon}_i = \varepsilon_i/mc\beta\gamma$.

Dispersion function

In curved systems, particles with different momenta p propagate at different horizontal orbits $\rho(s)$. The horizontal displacement function $\Delta x(s) = \rho(s) - \rho_0(s)$ a particle of momentum p experiences with respect to the reference orbit $\rho_0(s)$ — associated with the reference momentum p_0 — is usually expressed in terms of the “dispersion function” $D(s)$

$$\Delta x(s) = D(s)\frac{\Delta p}{p_0}\,, \qquad \Delta p = p - p_0\,. \tag{2.68}$$

The dispersion function $D(s)$ is a lattice-specific function of the the longitudinal path length s. In linear approximation, the trajectory equation for Δx in a curved system of variable bending radius $\rho_0(s)$ is given by [47]

$$(\Delta x)'' + \left(\kappa_x^2(s) - \frac{1}{\rho_0(s)}\right)\Delta x = \frac{1}{\rho_0(s)}\frac{\Delta p}{p_0}\,, \tag{2.69}$$

with $\kappa_x^2(s)$ the linear lattice function pertaining to the x direction which includes the linear part of the space-charge forces

$$\kappa_x^2(s) = k_x^2(s) - \frac{\frac{1}{2}K}{a(a+b)}\,. \tag{2.70}$$

Herein, K stands for the dimensionless generalized perveance, given for a beam current I and the particle charge $q = Ze_0$

$$K = \frac{2Ze_0 I}{4\pi\epsilon_0 mc^3\beta^3\gamma^3}\,. \tag{2.71}$$

For the sake of brevity, we use the notation $a^2(s) = \langle x^2 \rangle$ and $b^2(s) = \langle y^2 \rangle$ for the squares of the rms beam widths in the x- and y-directions, respectively. Inserting Eq. (2.68) into Eq. (2.69) yields the inhomogeneous equation of motion for $D(s)$

$$D''(s) + \left(\kappa_x^2(s) - \frac{1}{\rho_0(s)} \right) D(s) = \frac{1}{\rho_0(s)} \,. \tag{2.72}$$

Frequency slip factor

For straight systems, the time τ that is needed for a particle to cover a given distance C is determined by its velocity v only. The relation between τ and v is more complicated in a curved system since the path length C then depends on the particle velocity v

$$\tau = \frac{C(v)}{v} \,.$$

With the particle momentum $p = m\gamma v$ and $dC/C = d\rho/\rho$, we find the relations

$$\frac{d\tau}{\tau_0} = \frac{d\rho}{\rho_0} - \frac{dv}{v_0} \,, \qquad \frac{dv}{v_0} = \frac{1}{\gamma^2} \frac{dp}{p_0} \,,$$

hence

$$\frac{d\tau}{\tau_0} = \left(\frac{d\rho(s)}{\rho_0(s)} \bigg/ \frac{dp}{p_0} - \frac{1}{\gamma^2} \right) \frac{dp}{p_0} \,. \tag{2.73}$$

The dimensionless quantity $\alpha(s)$, given by the fractional change dC/C_0 of the path length C with respect to the fractional change dp/p_0 of the particle momentum is a lattice specific function

$$\alpha(s) = \frac{d\rho(s)}{\rho_0(s)} \bigg/ \frac{dp}{p_0} \,.$$

Its value after one turn, $\alpha(S)$, is commonly referred to as the "momentum compaction factor". From Eq. (2.73), we obtain the "frequency slip factor" $\eta(s)$, defined as the ratio of the fractional change $d\tau/\tau_0$ of the revolution time τ with dp/p_0 [37, 32]

$$\eta(s) = \alpha(s) - \frac{1}{\gamma^2} \,.$$

In order to derive the appropriate expression for the "longitudinal temperature" in a curved system, we must consider the velocity $\dot{s}$, defined as the velocity of the particle projection onto the reference orbit C_0

$$\dot{s} = \frac{C_0}{\tau} \qquad \dot{s}_0 \equiv v_0 \,.$$

With the identity $d\tau/\tau = -d\dot{s}/\dot{s}$, we find

$$dp = -\frac{m\gamma}{\eta(s)} \, d\dot{s} \,.$$

Therefore, the ratio $dp/d\dot{s}$ may be regarded as an "effective mass" m^* of a particle with a momentum deviation dp, as seen with respect to its relative motion to the reference particle on the reference orbit

$$m^* = \frac{dp}{d\dot{s}} = -\frac{m\gamma}{\eta(s)} \,. \tag{2.74}$$

Temperatures in the laboratory frame

For an unbunched beam, the temperature expression corresponding to Eq. (2.53) is given in the laboratory system by

$$m^* k_B T_{z,\ell} \equiv \left\langle (\Delta p)_\ell^2 \right\rangle ,$$

m^* denoting the effective mass, derived in Eq. (2.74). With the abbreviation $\delta^2(s) = \langle (\Delta p/p_0)^2 \rangle$, we may write the longitudinal temperature in the laboratory system as

$$k_B T_{z,\ell} = m\gamma c^2 \beta^2 |\eta(s)|\, \delta^2(s) . \tag{2.75}$$

In the temperature relaxation equation (2.62), this temperature quantifies the longitudinal momentum transfer due to collisions due to a spread of the velocity projections of the reference (center-of-mass) orbit. We must take the absolute value of $\eta(s)$ in Eq. (2.75) since — at least to first order — the roles of hitting particles and those being hit from behind are simply exchanged as $\eta(s)$ changes sign along the reference orbit.

The laboratory frame transverse temperature T_x is readily obtained from Eq. (2.53) and the trace-space emittance (2.67) as

$$k_B T_{x,\ell} = m\gamma c^2 \beta^2 \frac{\bar{\varepsilon}_x^2}{a^2} . \tag{2.76}$$

Obviously, the similar expression is obtained for $k_B T_{y,\ell}$.

Dispersion-related increase of horizontal beam width

As we have seen above, a particle encounters an additional displacement Δx with respect to the reference trajectory if its momentum deviates from the reference momentum. If the particle's horizontal displacement in the case of no momentum deviation is denoted by x_0, we get the total displacement as

$$x = x_0 + \Delta x .$$

This means for the horizontal second moment $\left\langle x^2 \right\rangle$

$$\begin{aligned} \left\langle x^2 \right\rangle &= \left\langle x_0^2 \right\rangle + \left\langle (\Delta x)^2 \right\rangle + \left\langle x_0 \Delta x \right\rangle \\ &= \left\langle x_0^2 \right\rangle + \left\langle (\Delta x)^2 \right\rangle , \end{aligned}$$

since the transverse oscillation ("betatron") amplitudes x_0 of all particles are not correlated with the dispersion-related deviations Δx. We may thus define

$$A(s) \equiv \sqrt{\langle x^2 \rangle} = \sqrt{a^2(s) + D^2(s)\delta^2}$$

as the dispersion-induced increased beam size $A(s)$ in the bending plane [48, 49] in the space-charge term of Eq. (2.70).

Friction number k_{fr}

For a longitudinally unmodulated beam, the real space particle density n contained in Eq. (2.66) may be expressed in terms of number of particles N per unit length s, and the maximum transverse beam widths $x_{\max} = 2a$ and $y_{\max} = 2b$

$$n = \frac{N/s}{\pi x_{\max}\, y_{\max}} ,$$

assuming a homogeneous transverse charge distribution. With the constant beam current I, the particle density n is obtained as

$$n = \frac{I}{4\pi Z e_0 c\beta\gamma^2\, ab}\,. \tag{2.77}$$

In our trace-space notation, the beam system friction coefficient β_{fr} must be replaced by the "friction number" $k_{\text{fr}} = \beta_{\text{fr}}/(c\beta\gamma)$ pertaining to the laboratory system. With the particle density (2.77) and the generalized perveance (2.71), the friction number k_{fr} follows from the friction coefficient (2.66) as

$$k_{\text{fr}} = \frac{K\,\beta}{3\sqrt{2\pi}}\,\frac{Z^2 r_c}{A\,ab}\left(\frac{k_B T_{\text{eq}}}{m\gamma c^2}\right)^{-3/2}\ln\Lambda\,.$$

Using the temperature expressions of Eqs. (2.75) and (2.76) for the longitudinal and the transverse temperatures in the laboratory system, we may again define the equilibrium temperatures T_{eq} as the arithmetic temperature average

$$\frac{k_B T_{\text{eq}}}{m\gamma c^2} = \tfrac{1}{3}\beta^2\left(\frac{\bar{\varepsilon}_x^2}{a^2} + \frac{\bar{\varepsilon}_y^2}{b^2} + |\eta|\delta^2\right)\,.$$

We thus finally get following representation of k_{fr}

$$k_{\text{fr}} = \frac{K}{3\sqrt{2\pi}\beta^2}\,\frac{Z^2 r_c}{A\,ab}\left[\frac{1}{3}\left(\frac{\bar{\varepsilon}_x^2}{a^2} + \frac{\bar{\varepsilon}_y^2}{b^2} + |\eta|\delta^2\right)\right]^{-3/2}\ln\Lambda\,.$$

In the vicinity of equilibrium, we may as well express T_{eq} as the *geometric* mean of the temperatures pertaining to the x, y, and z directions

$$\frac{k_B T_{\text{eq}}}{m\gamma c^2} = \beta^2\left(\frac{\bar{\varepsilon}_x^2}{a^2}\,\frac{\bar{\varepsilon}_y^2}{b^2}\,|\eta|\delta^2\right)^{1/3},$$

which leads to a simplified expression for k_{fr}

$$k_{\text{fr}} = \frac{K}{3\sqrt{2\pi}\beta^2}\,\frac{Z^2 r_c}{A}\,\frac{\ln\Lambda}{\bar{\varepsilon}_x\bar{\varepsilon}_y\sqrt{|\eta|}\delta}\,.$$

Coulomb logarithm

With the maximum impact parameter b_m, the Coulomb logarithm $\ln\Lambda$ is expressed as

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

$b_\perp$ denoting the impact parameter that corresponds to a 90° deflection [32], given by

$$b_\perp = \frac{Z^2 e_0^2}{4\pi\epsilon_0\, 3k_B T_{\text{eq}}}\,.$$

As usual for phenomena involving the long-range Coulomb forces, we must establish a reasonable upper limit for the maximum impact parameter b_m in order to keep Λ finite. In plasma physics, we usually identify $b_m \equiv \lambda_D$ with the Debye screening length. For non-neutralized systems, Jansen [9] suggested that we identify the maximum impact parameter b_m with the average distance between the particles ("ion sphere radius") rather than with the Debye screening length. The maximum impact parameter b_m can thus be expressed in terms of the average particle density n as $b_m \approx n^{-1/3}$. This means for $\ln\Lambda$

$$\ln\Lambda \approx \ln\frac{3k_B T_{\mathrm{eq}}}{Z^2 r_c\, mc^2\, n^{1/3}}\,. \tag{2.78}$$

Since β_{fr} depends only logarithmically on Λ, any result will not depend critically on the exact value of Λ. In the numerical estimations of intra-beam scattering effects, to be presented in Sec. 2.5, the Coulomb logarithm following form Eq. (2.78) evaluates to the usual value in the range of $\ln\Lambda \approx 20$. The inaccuracy in calculating the Coulomb logarithm is a general problem, which appears in all approaches on intra-beam scattering.

Coupled system of envelope and temperature relaxation equations

For the long-term beam dynamics in storage rings, we may disregard the transient effect of conversion of "free field energy" $W - W_{\mathrm{u}}$ into beam emittance, as described by Eq. (2.50). Neglecting the tiny residual emittance changes due to variations of the beams widths [50], the closed set of coupled equations for the envelopes, emittances, dispersion, and momentum spread finally reads

$$a'' + k_{\mathrm{fr}}a' + k_x^2(s)\,a - \frac{\frac{1}{2}K}{A(A+b)}a - \frac{\bar{\varepsilon}_x^2(s)}{a^3} = 0 \tag{2.79a}$$

$$b'' + k_{\mathrm{fr}}b' + k_y^2(s)\,b - \frac{\frac{1}{2}K}{A+b} - \frac{\bar{\varepsilon}_y^2(s)}{b^3} = 0 \tag{2.79b}$$

$$D'' + \left(k_x^2(s) - \frac{\frac{1}{2}K}{A(A+b)} - \frac{1}{\rho^2(s)}\right)D - \frac{1}{\rho(s)} = 0 \tag{2.79c}$$

$$\frac{1}{a^2}\frac{d}{ds}\bar{\varepsilon}_x^2 + \tfrac{2}{3}k_{\mathrm{fr}}\left(2\frac{\bar{\varepsilon}_x^2}{a^2} - \frac{\bar{\varepsilon}_y^2}{b^2} - |\eta(s)|\,\delta^2\right) = 0 \tag{2.79d}$$

$$\frac{1}{b^2}\frac{d}{ds}\bar{\varepsilon}_y^2 + \tfrac{2}{3}k_{\mathrm{fr}}\left(2\frac{\bar{\varepsilon}_y^2}{b^2} - \frac{\bar{\varepsilon}_x^2}{a^2} - |\eta(s)|\,\delta^2\right) = 0 \tag{2.79e}$$

$$|\eta(s)|\frac{d}{ds}\delta^2 + \tfrac{2}{3}k_{\mathrm{fr}}\left(2|\eta(s)|\,\delta^2 - \frac{\bar{\varepsilon}_x^2}{a^2} - \frac{\bar{\varepsilon}_y^2}{b^2}\right) = 0\,. \tag{2.79f}$$

If we add the temperature relaxation equations, i.e. the last three equations of the coupled set (2.79), we readily obtain

$$\frac{1}{a^2(s)}\frac{d}{ds}\bar{\varepsilon}_x^2(s) + \frac{1}{b^2(s)}\frac{d}{ds}\bar{\varepsilon}_y^2(s) + |\eta(s)|\,\frac{d}{ds}\delta^2(s) = 0\,. \tag{2.80}$$

Provided that the transverse beam sizes a, b, as well as the slip factor η may be regarded as adiabatic constants, Eq. (2.80) can be rewritten as

$$\frac{d}{ds}\left[\frac{\bar{\varepsilon}_x^2(s)}{a^2} + \frac{\bar{\varepsilon}_y^2(s)}{b^2} + |\eta|\,\delta^2(s)\right] = 0\,.$$

Integration leads to a constant of motion, first derived in a similar form by Piwinski [5]

$$\frac{\bar{\varepsilon}_x^2(s)}{a^2} + \frac{\bar{\varepsilon}_y^2(s)}{b^2} + |\eta|\,\delta^2(s) = \text{const.} \tag{2.81}$$

For real storage rings, this adiabatic invariant does *not* exist, as we cannot assume the transverse beam dimensions to be approximately constant along the focusing period. For this case, we must integrate the coupled set of equations (2.79) in order to determine the change of both the transverse emittances and the momentum spread due to intra-beam scattering effects. Since a temperature imbalance within the beam is periodically reestablished by the transverse focusing, no state of equilibrium, as suggested by (2.81), is ever reached. In terms of our approach, this means that the "temperature imbalance integrals" (2.64) can never vanish. Storage rings thus always generate a positive e-folding time τ_{ef} for the total beam emittance $\varepsilon_x \varepsilon_y \delta$, as given by Eq. (2.65).

We will present some examples of numerical solutions of the system (2.79) in the following section. Furthermore, the results will be compared to results of measurements in order to verify the accuracy of this approach to estimate intra-beam scattering effects.

2.5 Intra-beam scattering calculations for the Heidelberg Test Storage Ring (TSR)

2.5.1 Growth rates of emittance and momentum spread

The numerical integrations of the coupled set of equations (2.79) to be presented in the following are based on the lattice layout of the Heidelberg heavy ion storage ring TSR. For this ring, a systematic investigation of intra-beam scattering effects has been presented [51].

Figures 2.2 and 2.3 show two examples of numerical integrations of the coupled set of differential equations (2.79) for different initial beam conditions. The solid lines display the beam

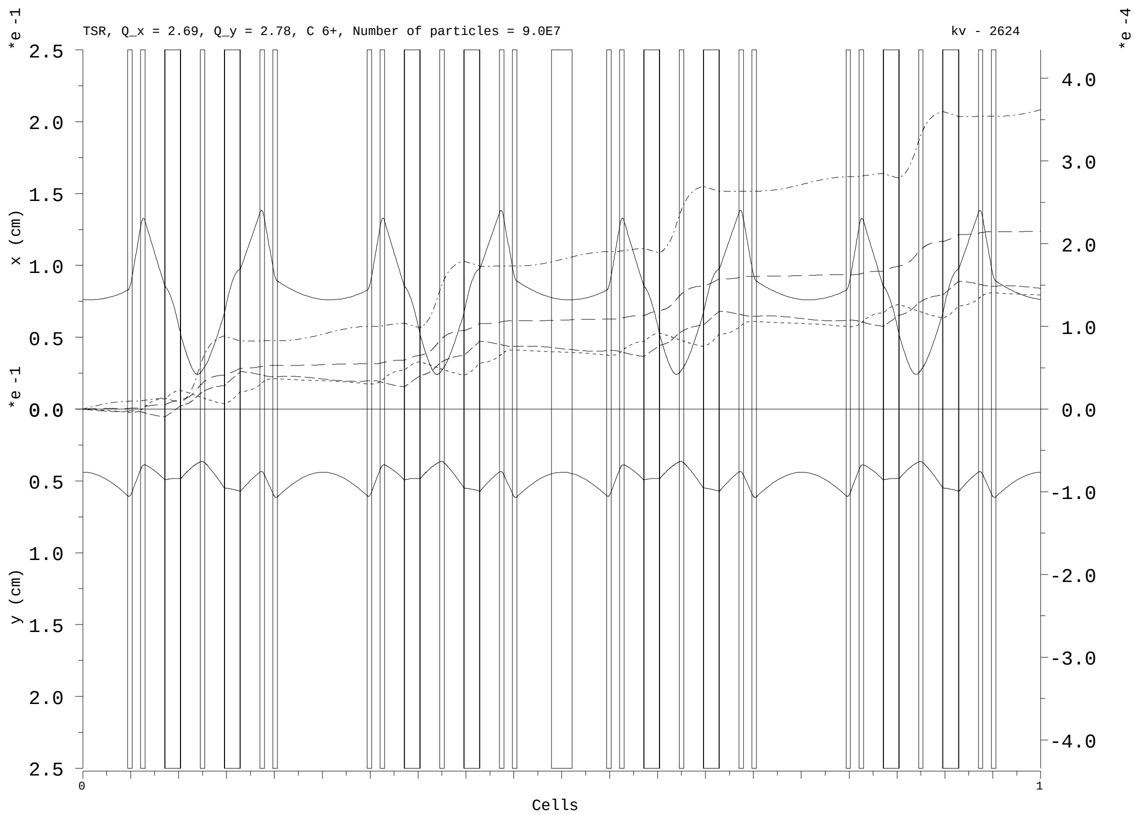

Figure 2.2: Beam envelopes (solid lines) and emittance and momentum spread growth factors (dashed lines) along one turn in the Heidelberg Test Storage Ring (TSR) for $Q_x = 2.69$ and $Q_y = 2.78$, $^{12}C^{6+}$ at 73.3 MeV. The scale on the right hand side applies to the dimensionless emittance and momentum spread growth functions.

envelopes in the horizontal and vertical directions representing a coasting (unbunched) beam that passes through the lattice of quadrupoles, bending magnets, and drift spaces. The dotted and the

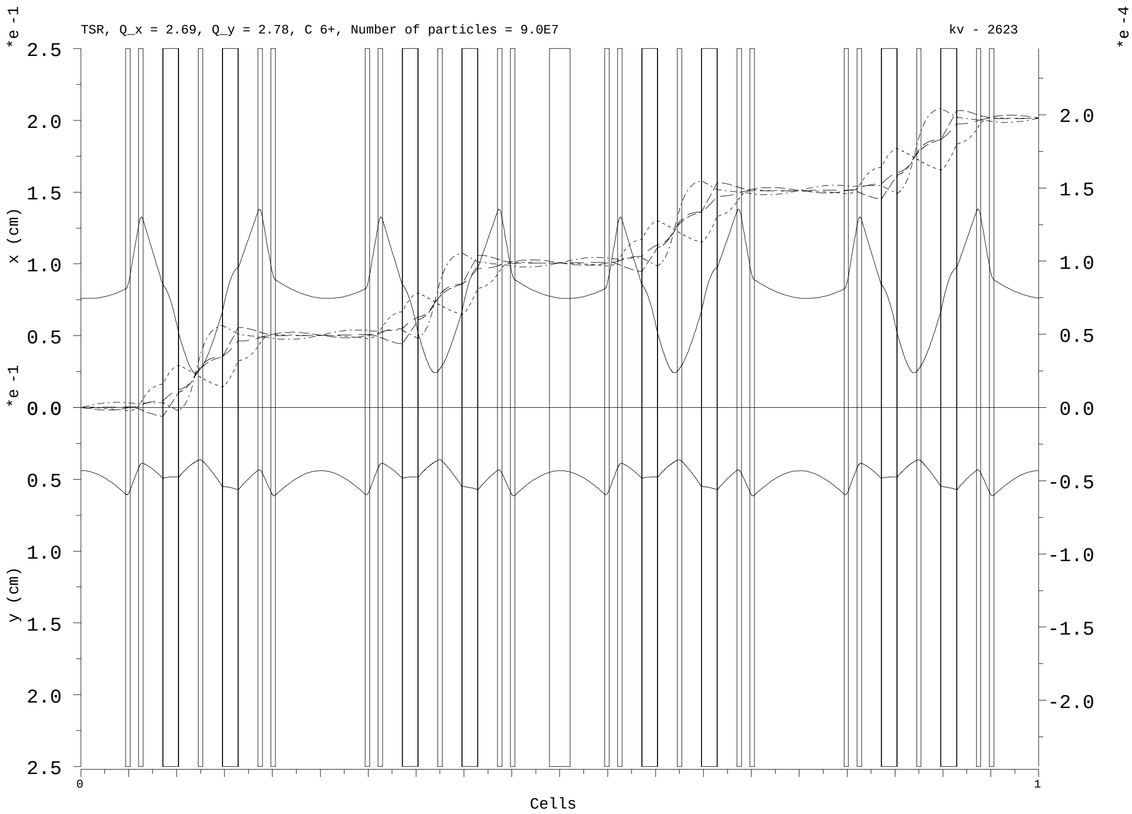

Figure 2.3: Beam envelopes (solid lines) and emittance and momentum spread growth factors (dashed lines) along one turn in the Heidelberg Test Storage Ring (TSR) for $Q_x = 2.69$ and $Q_y = 2.78$, $^{12}C^{6+}$ at 73.3 MeV. The initial emittances and momentum spread are adjusted to yield the minimum overall growth rate.

dashed lines show the emittance growth factors $(\bar{\varepsilon}_x(s)/\bar{\varepsilon}_x(0)) - 1$ and $(\bar{\varepsilon}_y(s)/\bar{\varepsilon}_y(0)) - 1$ along one turn, respectively. The dashed-dotted line displays the evolution of the rms momentum spread $(\delta(s)/\delta(0)) - 1$, whereas the long dashed line visualizes this growth rate for the total emittance $\bar{\varepsilon}_x \bar{\varepsilon}_x \delta$.

In Fig. 2.2, a sample integration is shown for an thermally unbalanced beam. As a consequence of the lack of temperature matching, the obtained growth rates differ in each degree of freedom.

Fig. 2.3 shows the similar case with the initial beam emittances and momentum spread being adjusted to yield a minimum average temperature anisotropy. This means that the "temperature imbalance integrals" (2.65) are minimized, and hence the overall emittance growth due to intra-beam scattering effects, as displayed by the long-dashed line.

2.5.2 Beam equilibria with cooling and comparison with measurements

The examples of the previous section display the instantaneous emittance and momentum spread growth rates for the particular initial conditions. Clearly, these initial conditions vary with time due to the continuous degradation of the beam quality due to intra-beam scattering. A comparison of the numerical results with measurements would be more accurate for a beam in a steady-state condition. In order to achieve a steady-state for a beam that is subject to non-negligible intra-beam scattering effects, we must apply an appropriate cooling mechanism [51] that exactly cancels the scattering related degradation of its quality. This situation is plotted in Fig.2.4.

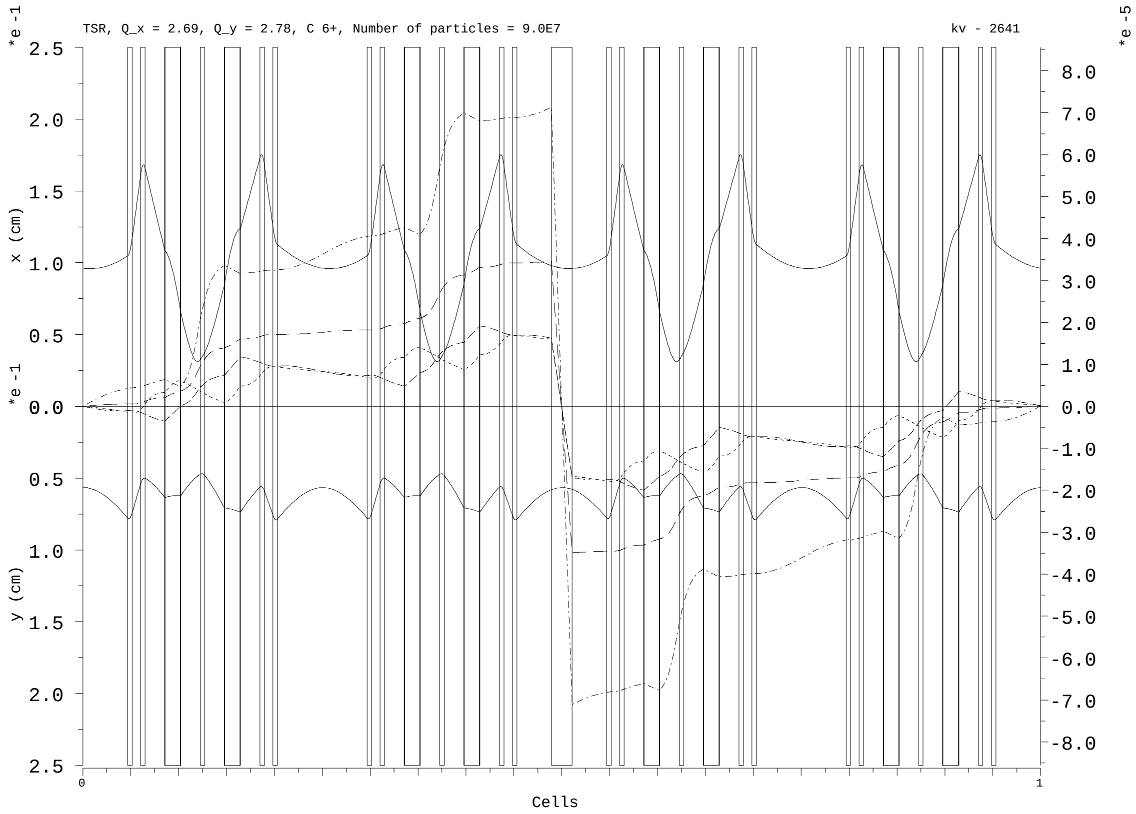

Figure 2.4: Beam envelopes (solid lines) and emittance and momentum spread growth factors (dashed lines) along one turn in the Heidelberg Test Storage Ring (TSR). The cooling section in the middle of the ring is now switched on.

The cooling rates were assumed as $1/\tau_{x,y} = 20\ \mathrm{s}^{-1}$ in the transverse directions, and $1/\tau_{\|} = 90\ \mathrm{s}^{-1}$ longitudinally. In the numerical calculations, the equilibrium emittances and momentum spread values for a given particle number and ring optics are obtained by adjusting appropriately the initial emittance and momentum spread settings. The comparison of the calculated equilibrium emittance and momentum spread values with the corresponding measurements are plotted in Fig. 2.5 for the case of C^{6+}, and for the single charged deuterium case in Fig. 2.6.

We observe that the calculated and the measured values of the momentum spread agree perfectly for C^{6+}. In all other cases, some deviation are obtained — as might be expected for our Fokker-Planck model of intra-beam scattering effects. In particular, a refined method to determine the appropriate Coulomb logarithm (2.78) could account for a better agreement. Furthermore, the model of friction and diffusion processes could be rendered more accurate [9] if the distinction is made between longitudinal and transverse friction and diffusion coefficients that describe the kinematics of the collisions. Of course, the emittance and momentum spread measurements themselves are inevitably associated with a considerable error. Also, the effective cooling rates surely depend one the number of stored ions — in contrast to our calculations presented here. Despite these discrepancies, the estimation of the intra-beam scattering related beam degradation with our model and its comparison with the corresponding measurements agrees within a factor of 2. This is the typical degree of accuracy that is encountered with various approaches on intra-beam scattering effects [32].

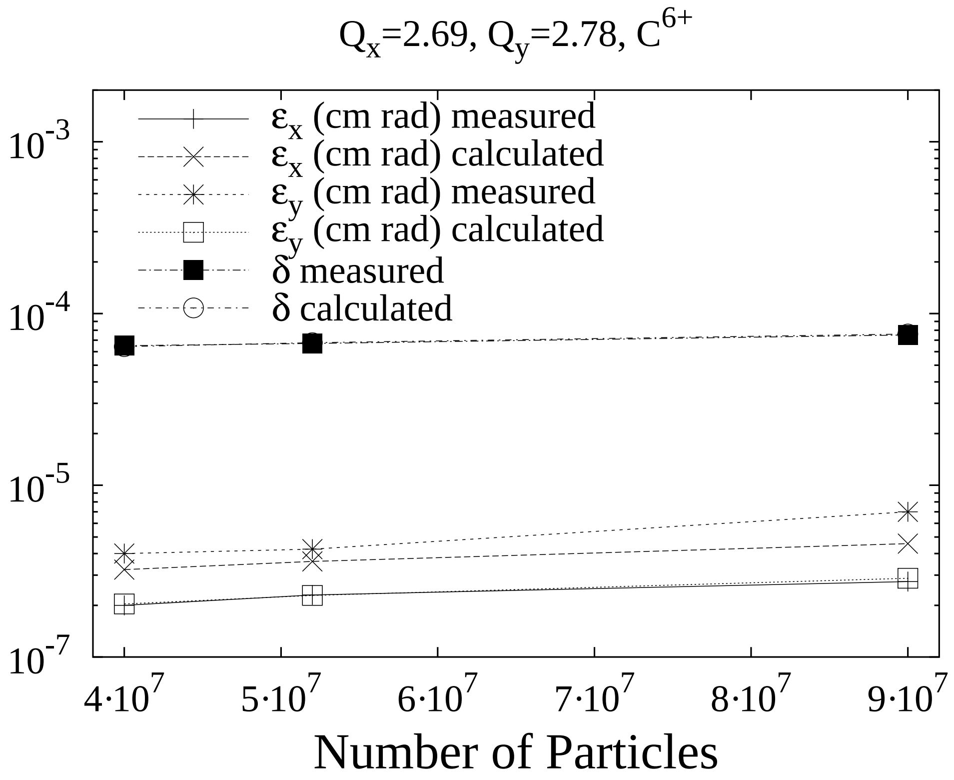

Figure 2.5: Comparison of the calculated equilibrium emittances and momentum spread with the corresponding measured quantities for C^{6+} at different numbers of stored ions.

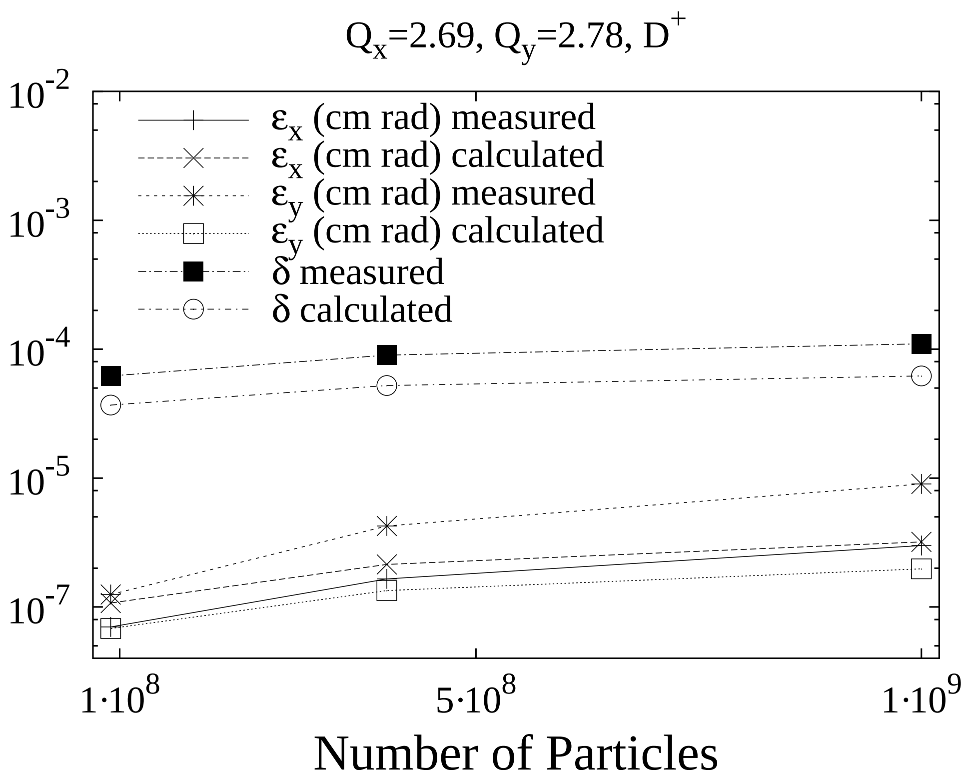

Figure 2.6: Comparison of the calculated equilibrium emittances and momentum spread with the corresponding measured quantities for D^{1+} at different numbers of stored ions.

Chapter 3

Numerical simulations of multi-particle systems

In this chapter, we make use of the results of the previous chapters in order to discuss the problem of “numerical noise” effects, emerging in numerical simulations of Hamiltonian systems of particles. With regard to an appropriate interpretation of the simulation results, we must distinguish two sources of errors that affect the validity of the obtained results.

For one, errors implicitly generated by the particular algorithm, designed to numerically integrate the particles’ equations of motion, must ensure the fundamental properties of a Hamiltonian system to be maintained. We will set up in the following the condition the simulation algorithm itself must fulfill in order to avoid an unphysical dilution of the phase space.

Furthermore, errors originating from the inherently limited accuracy of numerical methods may also limit the validity of the obtained simulation results. We will see that the Fokker-Planck approach — worked out in chapter 2 in order to analyze intra-beam scattering effects — may as well be applied to explain “numerical noise” phenomena in computer simulations. This will enable us to identify some results of our simulations as noise-related artifacts.

3.1 Symplectic maps

We now return to the deterministic description of the dynamics of n particle systems of chapter 1. Defining $\vec{x}$ as the $2n$ dimensional vector of all canonical variables

$$\vec{x} = \begin{pmatrix} q_1 \\ p_1 \\ \vdots \\ q_n \\ p_n \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{2n-1} \\ x_{2n} \end{pmatrix} ,$$

the set of canonical equations (1.2) that are derived from a Hamiltonian $H(\vec{x}, t)$ may be written equivalently as

$$\frac{d}{dt}\,\vec{x} = S\,\frac{\partial H}{\partial \vec{x}} ,$$

with S the $2n \times 2n$ symplectic characteristic matrix. We may write S as a $n \times n$ matrix of 2×2 generic characteristic matrices s_{ij}

$$S = \begin{pmatrix} s_{11} & \cdots & s_{1n} \\ \vdots & \ddots & \vdots \\ s_{n1} & \cdots & s_{nn} \end{pmatrix} , \qquad s_{ij} = \begin{pmatrix} 0 & \delta_{ij} \\ -\delta_{ij} & 0 \end{pmatrix} . \tag{3.1}$$

Herein, δ_{ij} denotes the Kronecker symbol. A general mapping $\mathcal{M}$ of the canonical variables

$$\mathcal{M} : \vec{x} \longmapsto \vec{x}\,' , \qquad \vec{x}\,' = \vec{f}(\vec{x})$$

is called *symplectic* if the Jacobi matrix M of $\mathcal{M}$, defined by

$$M = \left(\frac{\partial f_i}{\partial x_j} \right) , \qquad i, j = 1, \ldots, 2n$$

fulfills the condition

$$M^T S\, M = S \, , \tag{3.2}$$

with $M^T = (m_{ji})$ the transpose matrix of M. We will now show that all canonical transformations of the conjugate variables $(\vec{q}, \vec{p})$ are symplectic. As any finite canonical transformation can be expressed as an infinite sequence of infinitesimal canonical transformations, it is sufficient to consider the transformation derived from the infinitesimal canonical transformation $F_2(\vec{q}, \vec{p}, t)$, given by

$$F_2(\vec{q}, \vec{p}, t) = \sum_{i=1}^{n} q_i p_i' - \varepsilon\, G(\vec{q}, \vec{p}, t) \, . \tag{3.3}$$

The transformation rules for the canonical variables following from (3.3) are

$$q_i' = q_i - \varepsilon \, \frac{\partial G}{\partial p_i} \, , \qquad p_i' = p_i + \varepsilon \, \frac{\partial G}{\partial q_i} \, , \qquad i = 1, \ldots, n \, . \tag{3.4}$$

From Eq. (3.4), we directly obtain the Jacobi matrix M of the mapping $\mathcal{M}$ generated by F_2. Similar to the characteristic matrix S, defined by Eq. (3.1), the $2n \times 2n$ Jacobi matrix M can be written as a $n \times n$ matrix of "generic" 2×2 matrices m_{ij}

$$M = \begin{pmatrix} m_{11} & \ldots & m_{1n} \\ \vdots & \ddots & \vdots \\ m_{n1} & \ldots & m_{nn} \end{pmatrix} , \qquad m_{ij} = \begin{pmatrix} \delta_{ij} - \varepsilon \dfrac{\partial^2 G}{\partial p_i \partial q_j} & -\varepsilon \dfrac{\partial^2 G}{\partial p_i \partial p_j} \\[2ex] \varepsilon \dfrac{\partial^2 G}{\partial q_i \partial q_j} & \delta_{ij} + \varepsilon \dfrac{\partial^2 G}{\partial q_i \partial p_j} \end{pmatrix} . \tag{3.5}$$

With the matrices S and M, given by Eqs. (3.1) and (3.5), the matrix product $M^T S M$ can now be evaluated. Again, we easily convince ourselves that the resulting matrix can be written as a $n \times n$ matrix of "generic" 2×2 matrices $m_{ij}^T \, s_{ij} \, m_{ij}$

$$\begin{aligned} m_{ij}^T \, s_{ij} \, m_{ij} &= \begin{pmatrix} 0 & \delta_{ij} \\ -\delta_{ij} \left[1 - \varepsilon^2 \left\{ \dfrac{\partial^2 G}{\partial p_i^2} \dfrac{\partial^2 G}{\partial q_i^2} - \left(\dfrac{\partial^2 G}{\partial p_i q_i} \right)^2 \right\} \right] & 0 \end{pmatrix} \\ &= s_{ij} \qquad \text{to first order in } \varepsilon. \end{aligned}$$

We have thus shown that the canonical transformation that is defined by the general generating function (3.3) is symplectic to first order in ε — which is sufficient for infinitesimal transformations as any finite canonical transformation can be synthesized as an infinite concatenation of infinitesimal canonical transformations, in agreement with the formalism of section 1.6.1. As the time evolution of a Hamiltonian system itself establishes a particular canonical transformation, the mapping that represents the time evolution of a Hamiltonian system must be symplectic.

In computer simulations of dynamical N particle systems, this requirement must be met by the algorithm that pushes the system of particles forward in time. In particular, all intrinsic approximations that are necessary to limit the required computing times must maintain the symplectic nature of this mapping in order to avoid unphysical violations of Liouville's theorem (1.15), hence erroneous interpretations of the simulation results.

The time shift mapping usually consists of a sequence of elementary transformations, each of them representing a particular optical device along the beam line. Furthermore, the beam's continuously varying self-forces due to the Coulomb interaction of the beam particles are usually approximated by "kick maps" at fixed instants of time. Of course, each elementary transformations of its own must be symplectic in order to approximate the time evolution of the given Hamiltonian system. We will investigate in the following the implications of this condition for the examples of a finite quadrupole transformation and for a space-charge "kick" mapping.

3.1.1 Example 1: quadrupole transformation

For a one-degree-of-freedom Hamiltonian system, the Jacobi matrix associated with a canonical transformation is given by a 2×2 matrix M. The symplecticity condition (3.2) to be fulfilled by M writes explicitly

$$\begin{pmatrix} m_{11} & m_{21} \\ m_{12} & m_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \equiv \det M \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} , \tag{3.6}$$

which holds if and only if $\det M = m_{11}m_{22} - m_{12}m_{21}$ is unity

$$\det M = 1 \quad \Longleftrightarrow \quad M^T S M = S \, . \tag{3.7}$$

As has been shown in Sec. 1.1.3 in the context of Liouville's theorem, the determinant of M is indeed unity if the transformation is canonical. This means that the prove for symplecticity of a mapping of a one-degree-of-freedom system coincides with the task to show that the determinant of the related Jacobi matrix is unity.

The "hard edge" approximation of the quadrupole lens transformation (cf, for example, Lawson [37]), is given in the trace-space notation by

$$M = \begin{pmatrix} \cos kL & -k \sin kL \\ k^{-1} \sin kL & \cos kL \end{pmatrix} , \tag{3.8}$$

with L the longitudinal extension of the quadrupole field, and

$$k = \begin{cases} k_m & \text{in the focusing plane} \\ ik_m & \text{in the perpendicular plane} \end{cases} \quad , \quad k_m^2 = \frac{qB_0}{mc\beta\gamma a} \, ,$$

B_0 denoting the pole tip magnetic flux density, and a the aperture radius. Obviously, this linear model of a quadrupole transformation is associated with a unit determinant, hence fulfills the condition for symplecticity.

As a corollary, we may directly conclude that the drift transformation — following from (3.8) for the limit $k \to 0$ — is also symplectic.

The equivalence (3.7) does *not* hold anymore in general for systems with more than one degree of freedom. Setting up the symplecticity condition (3.2) for 4×4 matrices M and S, we easily find that symplectic matrices M have unit determinants, whereas $\det M = 1$ does not imply anymore M to be symplectic

$$M \;\text{ is symplectic} \;\; \Rightarrow \;\; \det M = 1 \, , \qquad \det M = 1 \;\; \not\Rightarrow \;\; M \;\text{ is symplectic} \, .$$

For mappings $\mathcal{M}$ that do not induce a coupling between the degrees of freedom, the $2n \times 2n$ Jacobi matrix can be decomposed into n independent 2×2 matrices. Then, of course, the mapping $\mathcal{M}$ is symplectic exactly if all 2×2 submatrices of M along the main diagonal have unit determinants.

3.1.2 Example 2: non-linear "space-charge kick" transformation

If the beam transformation only depends on the external optical devices, the particle equations of motion can be approximated by equations with piecewise constant coefficients. In the particular case of linear external forces, a solution matrix for each constant section exists. The particle mapping through the over-all system is then determined by the product matrix of all sections. This is no longer true if the particles' self-field cannot be neglected. Then, the forces acting on a particle are continuously varying along the longitudinal path s, as the beam's self-field depends on the phase-space location of all particles.

A frequently used algorithm to numerically integrate this class of equations of motion is referred to as the "leap-frog" method [52]. With this method, the finite transformation through a device of length $L = m\,\Delta L$ is divided into a sequence of m slices of length ΔL, respectively. The particle transformation through each slice consists of a lumped kick transformation $\mathcal{K}$, aiming to approximate the action of the continuously varying self-field over ΔL. The kick transformation $\mathcal{K}$ is centered within a pair of mappings $\mathcal{M}_{\Delta L/2}$. These mappings reach over one-half the slice length ΔL along the particular device without considering the self-field. Therefore, the mapping $\mathcal{M}_{\Delta L/2}$ is determined by the particular beam optical device only. This scheme is sketched in Fig. 3.1.

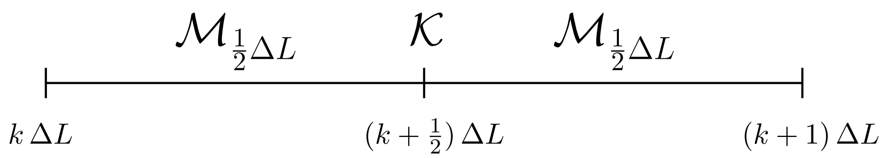

Figure 3.1: Schematic drawing of the sequence of transformations along one slice of a finite beam optical device. The lumped kick transformation $\mathcal{K}$, occurring at $(k+\frac{1}{2})\,\Delta L$, approximates the action of the continuously varying self-field along ΔL. The mappings $\mathcal{M}_{\Delta L/2}$ denote the transformations through fractions of length $\frac{1}{2}\Delta L$ of the external beam optical device without considering the self-field.

The magnitude of the momentum change a particle experiences due to the action of the self-field follows from the energy gain along the slice length ΔL. In terms of the trace-space notation referring to the laboratory frame, as introduced in Sec. 2.4.6, the change of the angular divergence with respect to the optical axis $\Delta \boldsymbol{x}_i'$ of particle i is obtained as

$$\Delta \boldsymbol{x}_i' = \frac{1}{mc^2\beta^2\gamma} \int\limits_{k\,\Delta L}^{(k+1)\,\Delta L} q\boldsymbol{E}_{\mathrm{sc},i}\big(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N,s\big)\,ds\,, \qquad i=1,\ldots,N\,. \tag{3.9}$$

As a further approximation, the continuously varying self-field $\boldsymbol{E}_{\mathrm{sc},i}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N,s)$ in (3.9) is replaced by the instantaneous field at $(k+\frac{1}{2})\Delta L$, assuming that the variation of this field along ΔL is negligible. Accordingly, the space-charge kick $\Delta \boldsymbol{x}_i'$ on particle i is determined by the simplified expression

$$\Delta \boldsymbol{x}_i' = \frac{\Delta L}{mc^2\beta^2\gamma} q\boldsymbol{E}_{\mathrm{sc},i}\big(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N,(k+\tfrac{1}{2})\Delta L\big)\,, \qquad i=1,\ldots,N\,. \tag{3.10}$$

As the lumped kick transformation does not push the particles forward along the beam axis, the particle positions $\boldsymbol{x}_i$ remain unchanged ($\Delta \boldsymbol{x}_i = 0$). Summarizing, the $6N$ particle coordinates before (b) and after (a) the kick transformation are given by

$$\boldsymbol{x}_i\big|_a = \boldsymbol{x}_i\big|_b \tag{3.11a}$$

$$\boldsymbol{x}_i'\big|_a = \boldsymbol{x}_i'\big|_b + \Delta\boldsymbol{x}_i'\big(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n\big)\,, \qquad i = 1,\ldots,N\,, \tag{3.11b}$$

with $\Delta\boldsymbol{x}_i'$ determined by Eq. (3.10). Setting up the Jacobi matrix M of the transformation (3.11), and evaluating the matrix product $M^T SM$, we straightforwardly convince ourselves that the lumped kick transformation (3.11) is indeed symplectic. We conclude that a beam transformation consisting of symplectic mappings $\mathcal{M}$ characterized by the particular beam optical devices and a sequence of lumped kick transformations $\mathcal{K}$ that approximate the continuously varying self-fields is also symplectic. For the simplest possible case, i.e. for $\mathcal{M}$ representing a drift transformation, the comparison with a Taylor expansion shows that the time-step error associated with the leap-frog algorithm [53] vanishes with $\mathcal{O}\big((\Delta L)^3\big)$.

3.2 "Numerical noise" effects in multi-particle computer simulations of beams

3.2.1 The emerging of irreversibility in multi-particle simulations

Owing to the fact that an analytical solution for the problem of particles interacting by Coulomb forces does not exist, computer simulations have become the tool of choice for the study of charged particle beams. A basic concept pursued in these simulations is to model the actual beam — usually consisting of a huge number N of particles — by a representative sample of a relatively small number of simulation particles $N^{\,\mathrm{sim}} \ll N$. This approximation ensures that the required computing resources of our simulations stick to a reasonable level. Explicitly, the coupled system of single particle equations of motion to be numerically integrated writes

$$m\ddot{\boldsymbol{x}}_i - \boldsymbol{F}_{\mathrm{ext}}(\boldsymbol{x}_i,t) - q\big(\boldsymbol{E}_i + \dot{\boldsymbol{x}}_i\times\boldsymbol{B}_i\big) = 0\,, \qquad i = 1,\ldots,N^{\,\mathrm{sim}}\,. \tag{3.12}$$

Again, $\boldsymbol{F}_{\mathrm{ext},i}$ denotes the force applied to the i-th particle by the external optical devices. Furthermore, $\boldsymbol{E}_i$ and $\boldsymbol{B}_i$ stand for the electric and magnetic self-fields acting on the beam. As the equation of motion (3.12) follows from a Hamiltonian (1.79), the mapping defined by the time integral of the coupled system (3.12) is symplectic. This property must be maintained by the numerical integration algorithm of the respective simulation code. Otherwise, if the simulation algorithm does not comply with the symplectic nature of the time evolution of a Hamiltonian system, the simulation results will generally not obey Liouville's theorem (1.15). As the consequence, we then encounter an unphysical dilution of the μ-phase-space volume filled by the simulation particles, resulting in an artificial growth of the beam's rms emittances $\varepsilon_{x,y,z}(t)$. Using symplectic integration algorithms to approximate the solution of the system (3.12) — as sketched in Sections 3.1.1 and 3.1.2 — we avoid a major cause for misleading simulation results. The emittance growth curves to be presented in the following were obtained on the basis of a symplectic integration technique.

Nevertheless, a non-symplectic integration technique is not the only source for unphysical effects to occur in numerical simulations of Hamiltonian systems. This will become manifest if we apply the time reversal transformation of Sec. 2.2.3

$$t\to -t\,,\qquad \boldsymbol{x}\to\boldsymbol{x}\,,\qquad \dot{\boldsymbol{x}}\to -\dot{\boldsymbol{x}} \tag{3.13}$$

to the system of equations of motion (3.12). Obviously, Eq. (3.12) does not change by virtue of the transformation (3.13), which means that the system described by (3.12) is *reversible*. On the other hand, computer simulations of dynamical systems are inevitably accompanied by noise-like errors originating in the generally limited accuracy of numerical methods. As numerical errors obviously do not depend on the direction of time flow, the noise-related effects are *not* reversed applying the transformation (3.13) to our simulation procedure. We conclude that the time evolution of the particle ensemble is rendered *irreversible* due to the limited accuracy of numerical methods. In other words, a computer simulation of our dynamical system (3.12) in fact provides a solution of a modified system that always comprises irreversible aspects.

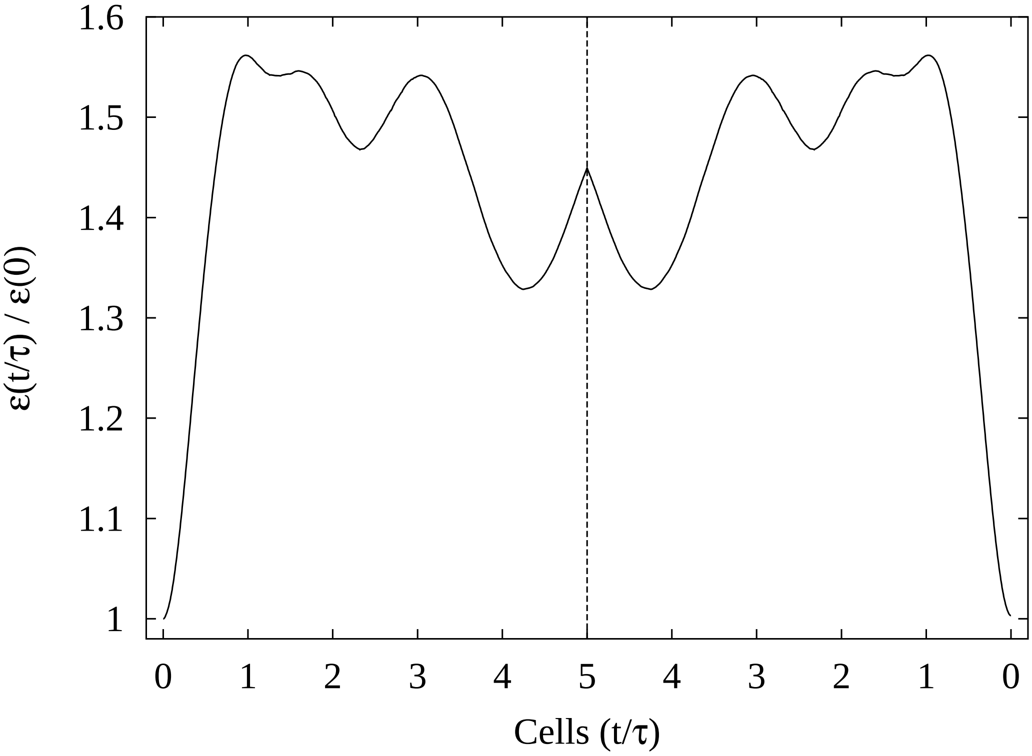

Figure 3.2: Emittance growth factors versus number of cells obtained for a non-stationary initial phase-space density at $\sigma_0 = 60°$, $\sigma = 15°$, 2500 simulation particles. The vertical dashed line marks the point of time reversal after 5 cells.

The emerging of irreversible effects in simulations of charged particle beams can be directly observed if we revert the direction of time flow in a computer simulation [54]. If a beam is injected in a non-equilibrium state into an ion optical system, the phase-space density f adapts itself rapidly to the external force field — on the time scale of some plasma periods — until an average equilibrium is reached. This process is accompanied by a change of the rms emittances, whose magnitude is described by Eq. (2.50). In the simulation displayed in Fig. 3.2, a space-charge dominated charged particle beam is transformed along 5 focusing periods forward in time. Subsequently, the time direction of the simulation is reversed, and the beam is transformed backwards to the starting position. We observe that the initial non-equilibrium state in terms of its initial emittance is recovered, which means that the simulation results appear to be in agreement with the reversible equation of motion (3.12).

But this is no longer the case if the forward transformation exceeds a certain number of periods. Figure 3.3 shows the emittance variations obtained from a simulation similar to the previous one, but now with the forward and the subsequent backward transformations extending over 20 focusing periods. Obviously, the initial state is not recovered anymore due to the accumulated action of numerical errors. This behavior shows that the simulation results no longer strictly comply with

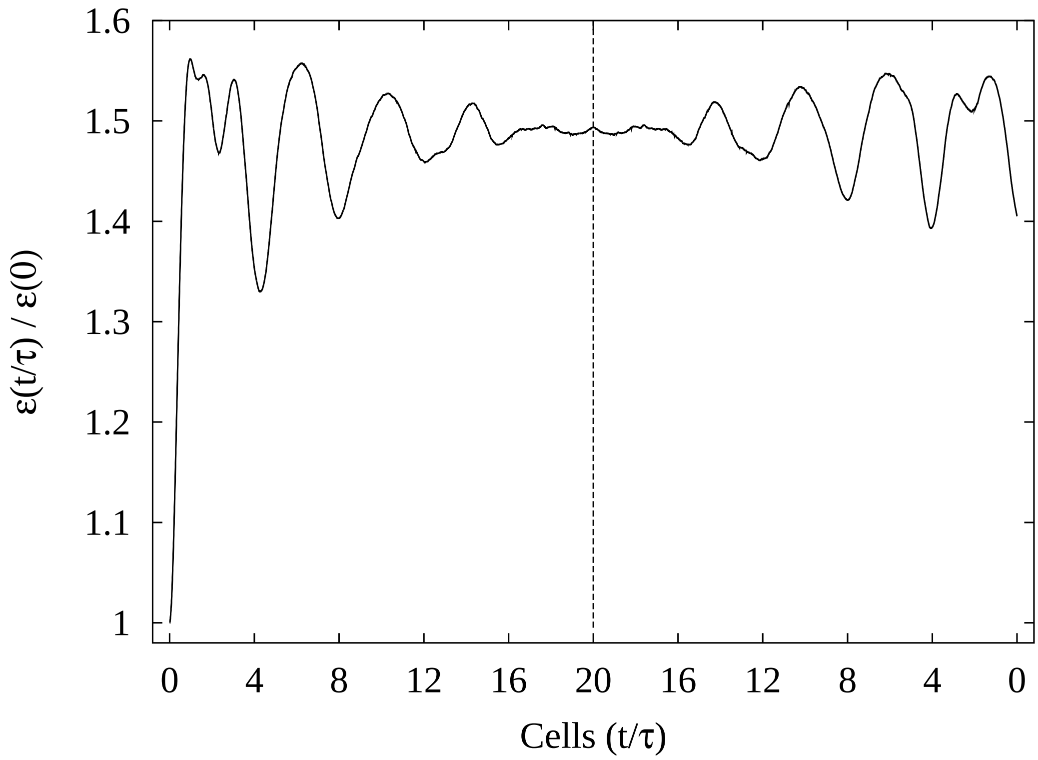

Figure 3.3: Emittance growth factors versus number of cells obtained for a non-stationary initial phase-space density at $\sigma_0 = 60°$, $\sigma = 15°$ per cell, 2500 simulation particles. The vertical dashed line marks the point of the time reversal after 20 cells.

the coupled set of equations of motion (3.12) — whose symplectic numerical integration is coded in the simulation algorithm.

A quantitative picture of the action of irreversible "numerical noise" effects is obtained from Fig. 3.4. This time, the direction of time integration of the single particle equations of motion (3.12) is reversed after 100 focusing periods (cells). For a small number of focusing periods — in this particular case for about 8 periods — we find an overlap of the emittance curves right before and after the time reversal. This reflects the reversible phase of the system's time evolution. Having exceeded this time span, the evolution of the system of interacting particles in rendered irreversible, indicated by the sharp change of sign of the emittance graph's slope. We observe that the emittance growth rate persisting during the irreversible phase of the back transformation exactly agrees with the growth rate encountered along the preceding forward transformation. This independence of the direction of time flow is exactly what we expect for an irreversible effect.

3.2.2 Fokker-Planck description of "numerical error" effects

As the starting point for an analytical treatment of "numerical noise" phenomena, we reconsider the generalized Fokker-Planck equation (2.43)

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m} \nabla_{\boldsymbol{x}} f + (\boldsymbol{F}_{\mathrm{ext}} + q\boldsymbol{E}_{\mathrm{sc}}) \nabla_{\boldsymbol{p}} f = \left[\frac{\partial f}{\partial t}\right]_{\mathrm{ir}} .$$

In this equation, the left-hand-side "Vlasov" terms describe the reversible aspects of the dynamics of a system of particles. The irreversible aspects are described within this model by the Fokker-

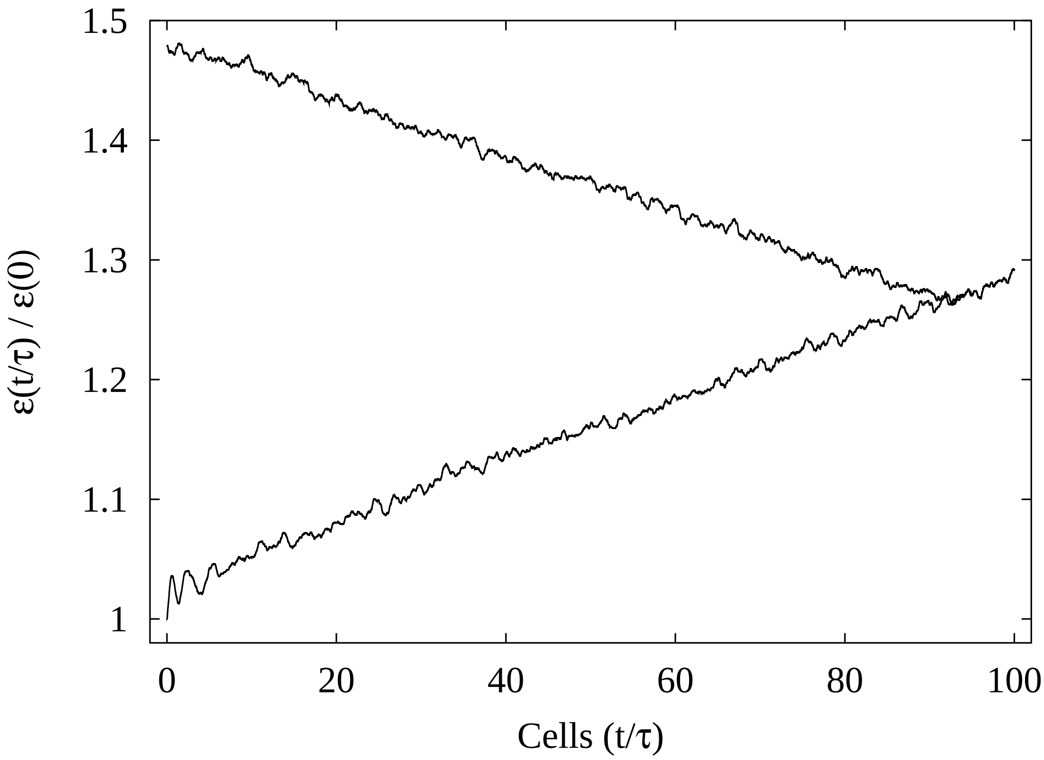

Figure 3.4: Emittance growth factors versus number of cells obtained by 3-D simulations of a periodic non-isotropic focusing system at $\sigma_0 = 60°$, $\sigma = 15°$ per cell, 2000 simulation particles. After 100 cells the time reversal occurs.

Planck equation

$$\left[\frac{\partial f}{\partial t}\right]_{\text{ir}} = -\sum_i \frac{\partial}{\partial p_i}\left[F_i^{\text{sim}}(\boldsymbol{p},t)\,f\right] + \sum_{i,j}\frac{\partial^2}{\partial p_i \partial p_j}\left[D_{ij}^{\text{sim}}(\boldsymbol{p},t)\,f\right] \ ,$$

with non-vanishing friction and momentum diffusion coefficients, F_i^{sim} and D_{ij}^{sim}, originating in the actual context from the "numerical noise" of the computer simulation. As has been shown is Sec. 2.2.3, this equation describes exactly those aspects of the time evolution of a dynamical system (3.12) that do *not* depend on the direction of time flow. Similar to intra-beam scattering phenomena within charged particle beams, the effects resulting from the limited numerical accuracy of the simulation particle dynamics are small compared to the action of all forces contained in the equation of motion (3.12).

The idea is to apply the mathematical framework of Sec. 2.3 to the description of noise-related effects simply by reinterpreting the respective Fokker-Planck coefficients. This approach appears justified taking into consideration that the gradual loss of information due to a large number of tiny numerical errors renders any memory of the system's state finite. In statistical physics, this class of systems is referred to as a Markov process [31]. Its equation of motion is given by the Fokker-Planck equation. As the consequence, we may use the subsequent equations (2.64) and (2.65) in order to estimate "numerical noise" phenomena occurring in our simulations. We recall that Eqs. (2.64) and (2.65) were derived from a moment analysis of the Vlasov-Fokker-Planck equation and the assumption that the stochastic process be isotropic. According to these equations, the e-folding time τ_{ef} of the total emittance $\varepsilon = \sqrt[3]{\varepsilon_x \varepsilon_y \varepsilon_z}$ was found to be given by

$$\tau_{\text{ef}}^{-1} = \tfrac{1}{9}\,\beta_{\text{fr}}^{\text{sim}}\left(I_{xy} + I_{xz} + I_{yz}\right) , \tag{2.64'}$$

with the "temperature imbalance integral" I_{xy} given by

$$I_{xy} = \frac{1}{T}\int_0^T \frac{\left[1 - r_{xy}(t)\right]^2}{r_{xy}(t)}\,dt \qquad , \qquad r_{xy}(t) = \frac{\varepsilon_y^2}{\langle y^2 \rangle}\frac{\langle x^2 \rangle}{\varepsilon_x^2}\,, \tag{2.65'}$$

and T denoting the period of the external force field. The similar definition applies for the coefficients I_{xz} and I_{yz}. Equation (2.64') states that the Fokker-Planck approach to model "numerical noise" effects inherent in our simulations predicts the time evolution of the emittances to depend on both a "simulation friction" coefficient $\beta_{\mathrm{fr}}^{\mathrm{sim}}$ and the detailed evolution of the temperature imbalances within the particle ensemble.

Comparing simulation runs for a given focusing lattice with different numbers N^{sim} of simulation particles, we implicitly vary $\beta_{\mathrm{fr}}^{\mathrm{sim}}$. At the same time, the temperature imbalances are kept constant. On the other hand, we may as well vary the underlying focusing lattice, thereby modifying the temperature imbalances. This time, we keep the number of simulation particles — hence $\beta_{\mathrm{fr}}^{\mathrm{sim}}$ — unchanged. In either case, specific growth rates of the emittances are to be expected according to Eq. (2.64'). We will show in Sections 3.2.4 and 3.2.5 that the emittance growth rates actually obtained in our simulations indeed follow these predictions. Beforehand, we will discuss the constituents of the friction coefficient $\beta_{\mathrm{fr}}^{\mathrm{sim}}$ in the realm of "numerical noise phenomena".

3.2.3 The friction coefficient for computer simulations

The emerging of "numerical noise" related effects can be visualized in the way that a weak "field" of non-Hamiltonian forces is superimposed on the Hamiltonian forces constituting the set of equations of motion (3.12). In the picture of a continuous description of particle dynamics, addressed in chapter 2, the action of non-Hamiltonian ("Langevin") forces causes the μ-phase-space Liouville theorem (2.4) to be violated. As these "non-Liouvillean" effects are actually small, we are allowed to approximate the dilution process of the μ-phase space in terms of the Fokker-Planck equation. With this approach, we condense the action of the non-Hamiltonian "noise forces" into non-vanishing friction and diffusion coefficients, F_i and D_{ij}, of the Fokker-Planck equation (2.43).

With the physical processes of friction and diffusion depending on each other, the respective Fokker-Planck coefficients are related by a fluctuation-dissipation theorem. For the idealized picture of an isotropic diffusion and friction process, this theorem is established by Einstein's relation (2.39). This relation obviously applies for irreversible "numerical noise" effects emerging in computer simulations of Hamiltonian systems, as these processes can indeed be regarded as isotropic. As the consequence, we are left with the simulation-specific friction coefficient $\beta_{\mathrm{fr}}^{\mathrm{sim}}$ as the only free parameter. The parameter $\beta_{\mathrm{fr}}^{\mathrm{sim}}$ thus characterizes globally to what extent a computer simulation of a Hamiltonian system actually lacks reversibility. Obviously, $\beta_{\mathrm{fr}}^{\mathrm{sim}}$ depends on the length of the floating point data representation and the number of floating point operations per unit time step. If the self-field of the particle ensemble is calculated by a Poisson solver that is based on a finite grid, the particular field interpolation algorithm will also contribute to some characteristic extent to the production of "numerical noise". Furthermore, the "susceptibility" of the dynamical system itself to the action of Langevin forces determines the time evolution of small deviations from a particular phase-space state. For a system with regular trajectories, small perturbations of the system's phase-space state will cause small oscillations around the unperturbed motion. On the other hand, systems with a chaotic evolution of the phase-space trajectories will force small perturbations to evolve into large deviations compared to the unperturbed state.

Because of these involved dependencies, we cannot expect to obtain a closed expression for the "simulation friction" coefficient $\beta_{\mathrm{fr}}^{\mathrm{sim}}$, similar to the friction coefficient (2.66) that has been worked out for the physical process of phase-space dilution due to intra-beam scattering. By comparing the long-term emittance growth rates encountered in simulation runs with different temperature imbalances (2.65’), we can determine the effective $\beta_{\text{fr}}^{\text{sim}}$ from the simulation results according to Eq. (2.64’).

3.2.4 Simulations based on a 2-dimensional beam model

The 2-dimensional x, y-beam model is widely used in analytical as well as in numerical approaches to the study of the transformation of unbunched (“coasting”) beams. We note that with regard to intra-beam scattering effects, the interaction with the longitudinal degree of freedom cannot be neglected. In other words, the 2-dimensional beam model is not adequate for the estimation of emittance growth effects due to intra-beam scattering. We will address this topic in the next section.

With the equilibrium temperature $T = \frac{1}{2}(T_x + T_y)$ for this beam model, Eq. (2.40) for the entropy change and Eq. (2.52) for the related irreversible emittance growth can be combined to yield

$$\frac{1}{k_B}\frac{dS}{dt} = \tfrac{1}{2}\beta_{\text{fr}}^{\text{sim}}\,\frac{d}{dt}\ln\varepsilon_\perp^2(t)\bigg|_{\text{ir}} = \tfrac{1}{2}\beta_{\text{fr}}^{\text{sim}}\,\frac{(T_x - T_y)^2}{T_x T_y}\,, \tag{3.14}$$

with $\varepsilon_\perp^2 = \varepsilon_x\varepsilon_y$ the product of the transverse rms emittances. Accordingly, beam transport without noise-related emittance growth, hence reversible beam propagation, appears possible if either

(1) $\beta_{\text{fr}}^{\text{sim}} \equiv 0$, or

(2) $T_x \equiv T_y\,.$

The first case represents the Vlasov description of beam dynamics, covered in section 2.3.2. By the entropy definition of Eq. (2.30), this approach is always associated with a vanishing growth of the entropy S.

The second case states that no degradation of the beam quality occurs, as long as no heat is transferred between the transverse degrees of freedom. This condition is met in the 2-dimensional beam model if we transform a matched beam through a continuous or interrupted solenoid channel.

Equation (3.14) indeed explains the results of computer simulations that are based on the 2-dimensional beam model. The upper three curves in Fig. 3.5 show the evolution of the rms emittance growth factors along a quadrupole channel, as they were obtained for different numbers of simulation particles, while all other simulation parameters were kept unchanged. In all cases, the beam is launched with a self-consistent water-bag distribution [55, 56, 42] as the initial phase-space state. The external focusing has been approximated by strictly linear forces and the hard edge lens model. With the space-charge forces being approximated by lumped “kick” transformations, the simulation algorithm is strictly symplectic, according to the results of Sections (3.1.1) and (3.1.2). Under these circumstances, the overall emittance growth must be attributed to the action of Langevin forces generated by the “numerical noise” that inevitably accompany our simulation process. We observe that the overall growth rates as well as the amplitude of the local emittance fluctuations strongly depend on the number of particles used in the simulation. This growth cannot saturate as the temperature imbalance ratio I_{xy} is continuously restored by the external focusing forces along the lattice. With regard to Eq. (3.14), we conclude that the Langevin forces induce a finite “simulation friction coefficient” $\beta_{\text{fr}}^{\text{sim}}$, which is, to first order, inversely proportional to the number of simulation particles.

The justification to use Eq. (3.14) in order to explain the emittance growth encountered in our simulations is further confirmed by the simulation results displayed in the lower curve of Fig. 3.5. It shows the evolution of the rms emittance growth factors during the propagation of a matched beam through a periodic solenoid channel. As the beam stays circular symmetric along the entire channel ($T_x \equiv T_y$), no transverse temperature gradient exists. Then, according to Eq. (3.14), no overall growth of the emittance is to be expected. We observe that the emittance fluctuations

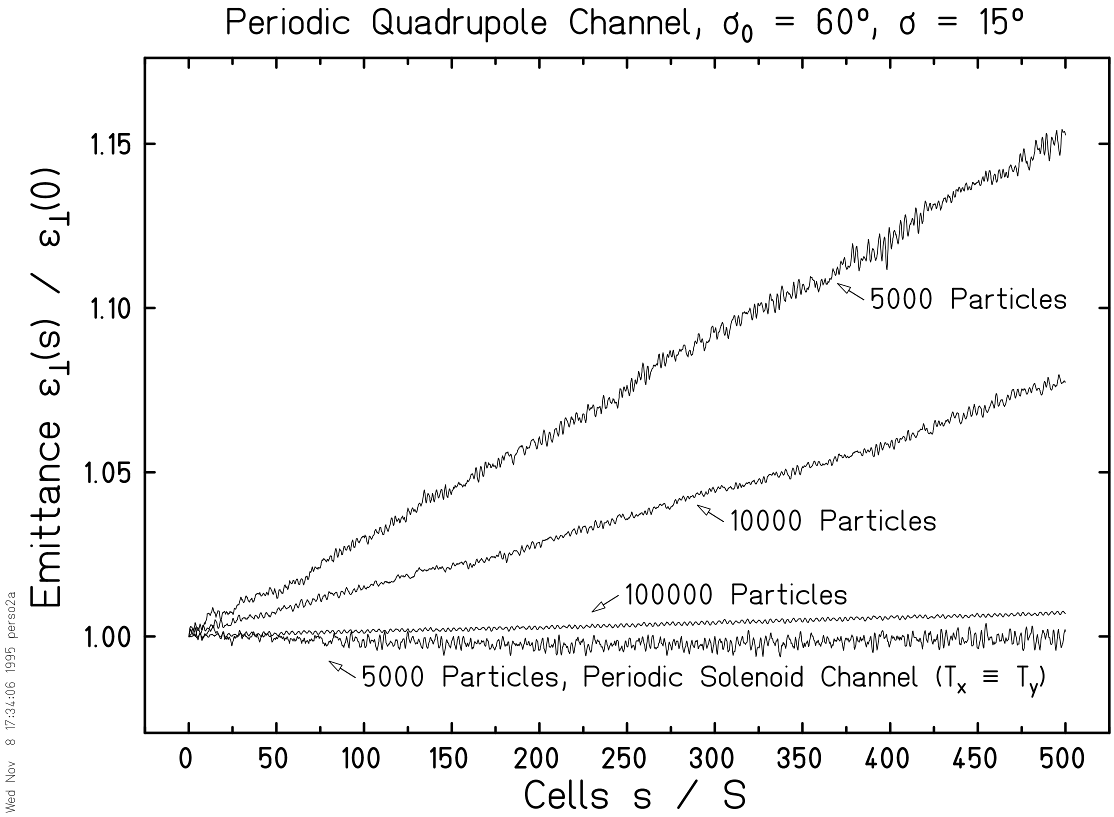

Figure 3.5: Emittance growth factors versus number of cells obtained by 2-dimensional particle-in-cell simulations of beam transport channels at $\sigma_0 = 60°$, $\sigma = 15°$. The upper three curves display the results of quadrupole channel simulations with different numbers of simulation particles. For comparison, the lowest curve shows the emittance growth factors of a periodic solenoid channel simulation.

are similar in amplitude to those in the quadrupole channel simulation performed with the same number of simulation particles. This means that in both cases the fluctuating part of the self-fields impose a similar "simulation friction coefficient" $\beta_{\mathrm{fr}}^{\mathrm{sim}}$. Yet, due to the lack of temperature differences, these fluctuations indeed do *not* produce an overall increase of the rms emittance, as suggested by Eq. (3.14).

3.2.5 3-dimensional beam simulation

Figure 3.6 displays emittance growth factors obtained for simulations of beam transport through fictitious lattices that focus the beam in all three spatial directions. In these simulations, *identical* beams, i.e. beams possessing the same particle species, energy, number of particles, emittance values and phase-space density profiles are transformed through *equivalent* transport channels. The lattices differ solely in the type of focusing necessary to sustain the average beam width but produce the same zero current tune σ_0 and depressed tune σ, respectively. Of course, the time step width used in our simulations as well as the algorithm to determine self-fields of the beam must be the same for all three kinds of transport channels.

Owing to the low number of simulation particles, significant emittance fluctuations occur even in the "equilibrium" case of a beam propagating through a continuous isotropic focusing channel. In order to isolate clearly the emittance growth effects that may be attributed to the non-continuous focusing, we divide the respective emittances ε by the emittances $\varepsilon^{\mathrm{cif}}$ obtained for the equivalent continuous isotropic focusing channel. This means that the growth factors pertaining to the contin-

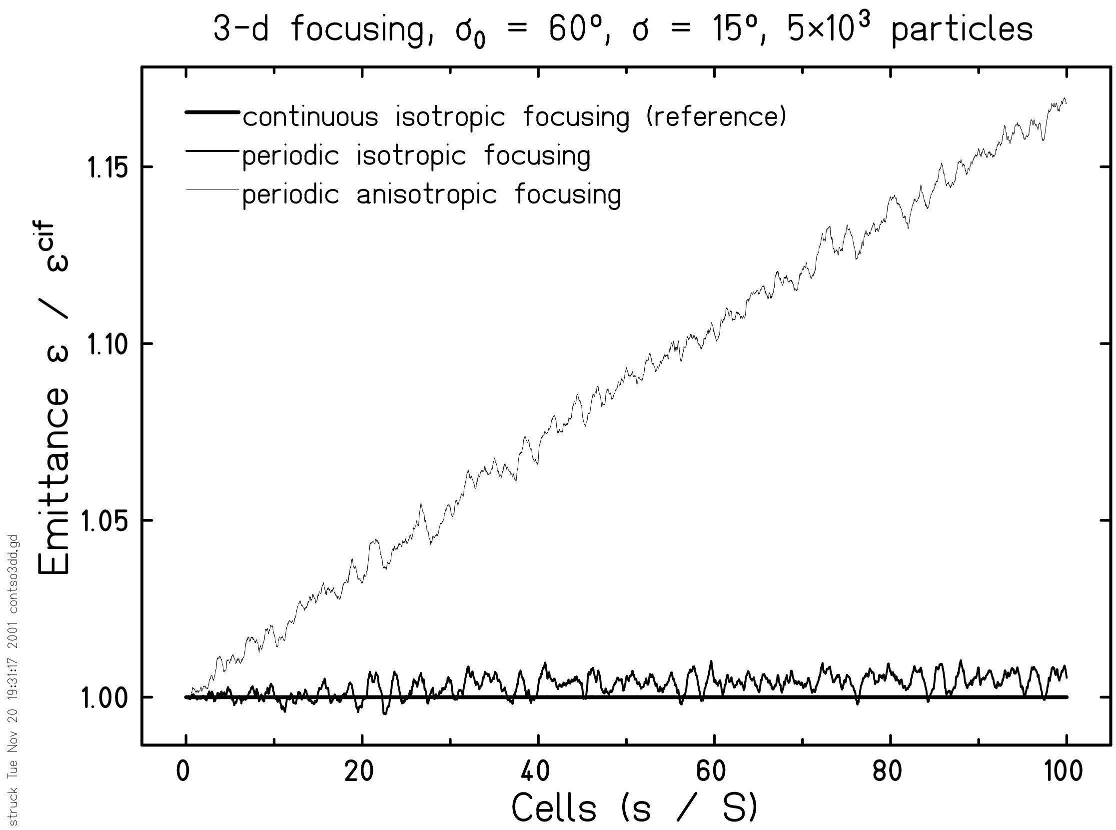

Figure 3.6: Emittance growth factors versus number of cells obtained by 3-dimensional simulations of beam transport channels at $\sigma_0 = 60°$, $\sigma = 15°$, and 5×10^3 simulation particles. The plotted growth factors refer to the purely statistical growth factors encountered for the transformation through a continuous and isotropic focusing (cif) channel.

uous channel are taken as reference values for the growth factors of the periodic focusing channels. Consequently the emittance growth curve for the continuous channel appears as a horizontal line in Fig. 3.6.

For the anisotropic focusing channel, we observe a monotonous, non-saturating behavior of the obtained emittance growth values. This is exactly what we expect if we recall Eq. (2.64). Due to the anisotropic focusing, a non-vanishing beam temperature imbalance along the lattice is enforced, leading to a finite anisotropy coefficient (2.65). With regard to Eq. (2.64'), this means that both quantities, the finite temperature anisotropies I_{ij} as well as the non-vanishing effective friction coefficient $\beta_{\text{fr}}^{\text{sim}}$ induce a specific irreversible growth rate of the beam emittance according to Eq. (2.64).

For a comparison, Fig. 3.6 displays in addition the growth rates from the simulation of a matched beam that is transformed through a equivalent periodic isotropic focusing channel. This means that the periodic focusing is accomplished in a way to keep the beam temperatures balanced throughout the channel. Consequently, the “temperature imbalance integrals” (2.65') are zero — apart from statistical effects. We observe that an almost negligible growth of the rms emittance is observed in this simulation. This outcome is again explained by Eq. (2.64'), which states that even a positive $\beta_{\text{fr}}^{\text{sim}}$ does not cause an increase of the rms emittance if the integrals (2.65') vanish. The residual emittance growth may be attributed to deviations from a ideal beam symmetry due to the low number of simulation particles. Furthermore, the approximation (2.55) for the equilibrium temperature holds exactly in the idealized case of δ-correlated noise forces (2.16) only.

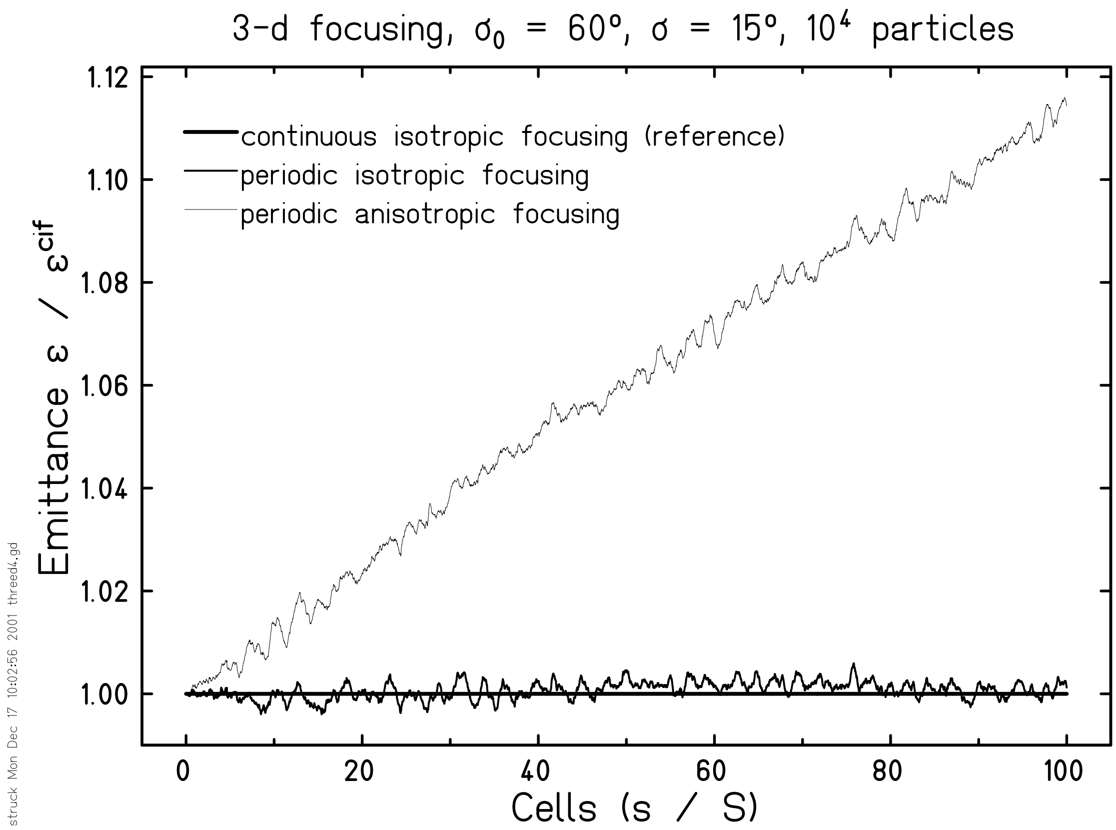

Figure 3.7: Emittance growth factors versus number of cells obtained by 3-dimensional simulations of beam transport channels with the parameters of Fig 3.6. The number of simulation particles has been scaled up to 10^4.

In Fig. 3.7, the similar calculations are displayed with an increased number of simulation particles (10^4). We observe that the slope of the emittance growth for the anisotropic focusing channel is now significantly smaller. At the same time, the amplitudes of the local emittance fluctuations are also reduced. As the variation of the number of simulation particles does not modify the temperatures imbalances (2.65'), we conclude that a smaller numerical friction coefficient $\beta_{\mathrm{fr}}^{\mathrm{sim}}$ accounts for the reduced emittance growth rate for the periodic anisotropic focusing channel, as compared to the corresponding simulation results of Fig. 3.6. The small residual growth of the overall emittance, encountered in the previous case for the periodic isotropic beam modulation, has now completely vanished — which is exactly the expected result for zero temperature imbalances.

Summarizing, we find that numerical noise phenomena occurring in computer simulations of charged particle beams can adequately be described by the Fokker-Planck approach. For long-term simulations, the Fokker-Planck analysis provides the indispensable framework for an appropriate interpretation of simulation results of Hamiltonian systems.

Conclusions and outlook

A fairly general result has been found: a conserved quantity can straightforwardly be deduced for general non-linear and explicitly time-dependent Hamiltonian systems. The invariant has been derived in two different ways, namely as the result of an extended phase-space canonical transformation, and on the basis of Noether's theorem [2]. Our invariant thus embodies exactly the conserved quantity that emerges as the result of Noether's symmetry transformation. The invariant contains an unknown function $\xi(t)$ and its first and second time derivatives, which is determined by a linear homogeneous third-order auxiliary differential equation. In general, this auxiliary equation depends on the system's spatial degrees of freedom. Under these circumstances, the solution $\xi(t)$ can only be determined integrating the auxiliary equation *simultaneously* with the equations of motion. The invariant can be regarded as the conserved global energy for non-autonomous systems, which is obtained if we add to the time-varying energy represented by the Hamiltonian H the energies fed into or detracted from the system.

The existence of an invariant I has been shown to be useful to check the accuracy of numerical simulations of explicitly time-dependent Hamiltonian systems. Having numerically integrated the equations of motion, the system's third-order auxiliary differential equation can be integrated, and the numerical value of the "invariant" $I^{\,\mathrm{sim}}(t)$ can be calculated subsequently. The relative deviation $(I^{\,\mathrm{sim}}(t)-I(0))/I(0)$ from the exact invariant $I(0)$ can then be used as a global measure for the accuracy of the respective simulation.

Under certain conditions, the solutions $\xi(t)$ of the auxiliary equation may become unstable. Then, the hyper-surface of constant I becomes more and more distorted as $\xi(t)$ and its derivatives diverge. This may indicate a transition from a regular to a chaotic motion of the beam particles. Nevertheless, the physical implications that are associated with an unstable remain to be investigated.

It has been shown that the solution function $\xi(t)$ of the auxiliary equation remains non-negative for linear isotropic systems. In these cases, $\xi(t)$ may be interpreted as an amplitude function of the particle motion [57]. For all other Hamiltonian systems, the auxiliary function $\xi(t)$ may become negative. A connection between theses solutions of the auxiliary equation and the characteristics of the solutions of the equations of motion has not yet been established. Of course, the invariant I of the explicitly time-dependent system exists independently of the sign of $\xi(t)$. Yet, for negative $\xi(t)$, the elements of coordinate transformation matrix (1.22) become imaginary. This means that the evolution of the explicitly time-dependent Hamiltonian system can no longer be correlated to the dynamics of a time-independent system. Again, this might indicate a transition to a non-regular time evolution. A possible application would be to identify the parameter range of storage rings that are eligible for the formation of a beam halo. In any case, as $\xi(t)$ follows from the collective properties of the particle ensemble, its complete understanding should provide us with interesting and important insight into the system's dynamics.

For systems with a huge number of degrees of freedom, the individual particle approach, pursued in Chapter 1, is no longer appropriate. On the other hand, switching to a continuous description on the basis of a phase-space probability density means to smooth out all aspects that reflect the system's granular nature. For the realm of charged particle beams, we have shown in Chapter 2 that the Fokker-Planck equation provides a useful starting point for analytical approaches that include effects originating in the actual charge granularity. The second-order moment analysis of the Fokker-Planck equation may be applied to derive a set of equations that are directly related to the beam parameters. It follows that the emittance growth rates due to intra-beam scattering effects are related to both the temperature imbalances along the focusing lattice, and a global friction coefficient β_{fr}. The determination of the friction coefficient β_{fr}, in particular the appropriate choice of the Coulomb logarithm from the beam parameters, needs careful examination for each particular case. In a comparison with measured equilibrium emittances from the Heidelberg Test Storage Ring (TSR), we have shown the results of our model to agree within the range of a factor of 2.

The assumption that the diffusion process in velocity space is isotropic should be dropped in a refined treatment of our moment analysis of the Fokker-Planck equation. Of course, this means that the fluctuation-dissipation theorem in the form of the Einstein relation [36] no longer applies. As the result of a more accurate analysis, the accuracy of our estimation of intra-beam scattering effects can be expected to be significantly enhanced.

In Chapter 3, we have demonstrated the emerging of irreversibility in computer simulations of systems of particles due to “numerical noise” effects. Again, the Fokker-Planck equation was used as the basis for a quantitative description. Its moment analysis predicts that the noise-related emittance growth rates in simulations of charged particle beams should depend on both the magnitude of the noise force, and the average temperature anisotropy the beam experiences along the focusing lattice. Computer simulations of beam transport have been performed for various focusing lattices and numbers of simulation particles. The emittance growth rates encountered in these simulations indeed follow the predictions of the Fokker-Planck model. Emittance growth effects did not appear in cases where the temperature anisotropy within the system is negligible — even if the “computer noise” related forces are large. On the other hand, the emittance growth rates observed in systems with finite temperature anisotropy have been shown to strongly depend on the number of simulation particles, hence on the magnitude of the “noise forces”. The mysterious long-term growth of the emittance, as seen for a long time in simulations of beam transport systems, could thus be identified as a “computer noise” artifact.

Discreteness errors inevitably emerge in computer simulations of dynamical systems. Therefore, the actual time evolution of the simulated system always encloses irreversible aspects — even if the actually coded equations of motion are strictly reversible. In that sense, the simulation results can be regarded as exact solutions of a modified dynamical system that always comprises Langevin force terms. With the Fokker-Planck description of microscopic “computer noise” effects, we are able to understand its macroscopic consequences and thereby avoid misinterpretations of our simulation results. A systematic study that relates the magnitude of “numerical noise” effects to both the system’s enhanced granularity induced by the concept of “representative samples” of particles and the number of floating point operations is still outstanding.

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