Concept of entropy in the realm of charged particle beams

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Stochastic phenomena occurring within charged particle beams can be handled using the Vlasov-Fokker-Planck generalization of the Vlasov equation. In particular, this nondeterministic approach can deal with effects due to Coulomb scattering between the beam particles. Moreover, stochastic phenomena also occur in computer simulations of charged particle beams. Both processes—although different in their physical nature—can be described by the Vlasov-Fokker-Planck equation, since in both cases the underlying stochastic process can be classified as a Markov process. This description is applied to beams in periodic focusing systems. We derive an equation relating the change of the μ-phase space entropy to the change of rms emittance and ''temperature weighted excess field energy.'' This equation enables us both to improve our capability to interpret the results of computer simulations, as well as to identify the conditions needed to minimize scattering induced degradation of the quality of beams circulating in storage rings. [S1063-651X(96)06907-3]

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I. INTRODUCTION

Analytical approaches to particle motion that are based on the Vlasov equation require that Liouville theorem—though strictly valid only in the $6N$-dimensional Γ-phase space—also applies to the six-dimensional μ-phase space, at least to a good approximation. This is obviously correct in a regime where the motion of single particles can be treated as being independent of each other. In the more realistic case of interacting particles, the Liouville theorem remains fulfilled in the μ-phase space as long as the space charge fields can be regarded as smooth macroscopic functions. This is no longer true for cases where forces between individual particles play a role. One example for this ''non-Liouvillean'' behavior is the scattering induced emittance growth effect within ion beams (''intrabeam scattering''). A second example is the appearance of numerical noise phenomena in computer simulations of charged particle beams. As will be demonstrated in this article, the main source for this computer artifact originates in the modeling of a real beam, for performance reasons, by a ''simulation'' beam containing several orders of magnitude fewer particles.

In order to analyze non-Liouvillean phenomena, a generalization of the Vlasov equation becomes necessary. In this article we follow the approach applied earlier by Chandrasekhar [1], who modeled the non-Liouvillean contributions to the dynamics of particles by the Fokker-Planck equation [2]. The basis as well as the limitation of this model is the assumption that the process governing the non-Liouvillean effects is Markovian. The conditions under which the Fokker-Planck approach can be applied to the realm of ion optics has been discussed in earlier papers [3,4].

We will try to extend this ansatz in the following by introducing an entropy [5] in a way that directly relates it to the μ-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 in Sec. III that the so-defined entropy remains conserved as long as the μ-phase space Liouville theorem is fulfilled. Entropy changes thus directly reflect the occurrence of non-Liouvillean effects–which in turn will be described by the Fokker-Planck equation. This is the basis on which, in Sec. IV, the time derivative of the entropy will be calculated assuming that the beam's velocity distribution is Maxwellian.

For a special class of Markov processes—namely, for so-called Ornstein-Uhlenbeck processes [2]—this expression may be considerably simplified. As demonstrated in Sec. V, only *constant* Fokker-Planck coefficients are then contained in the equation for the change of entropy. We may restrict ourselves to the Ornstein-Uhlenbeck model if the non-Liouvillean part of the dynamics is small compared to that conserving the μ-phase space volume. This is always true for charged particle beam optics.

If the Fokker-Planck coefficients appertaining to each degree of freedom do not differ significantly from each other so that the diffusion and friction processes can be regarded as approximately isotropic, we may set up the fluctuation-dissipation theorem in its simplest form. This was first done by Einstein [6], in his work on the Brownian motion of particles. It is obviously valid in situations not too far from a fictitious thermodynamic equilibrium. We will show that entropy growth is then directly related to heat transfers between different degrees of freedom within the beam.

In Sec. VI we switch back to a more general treatment and we first of all review the idea of a moment analysis of the Vlasov-Fokker-Planck equation [7,8,4]. We are then prepared to set up the equation that relates entropy growth to changes of the rms emittance in conjunction with changes of the ''excess field energy.'' In this context, the known equation relating changes of the rms emittance to changes of the ''excess field energy''—first derived by Wangler [9]—appears as a special case.

In the last section, the entropy equation is applied to one- and two-dimensional (2D) beam models commonly used as simplifying concepts in the theory of charged particle beams. The well known phenomenon that simulations of periodic quadrupoles channels always exhibit—in contrast to solenoid channels—a specific increase of the rms emittance is then easily explained and identified as a computer noise artifact.

Furthermore, a scaling law for intrabeam scattering effects in real (three-dimensional) beams is obtained. It states that the emittance growth rates are determined both by the general beam parameters as well as by the particular optics of the beam transport system.

II. THE ENTROPY CONCEPT

We start our analysis by defining the six-dimensional normalized μ-phase space density function

$$f = f(x,y,z,p_x,p_y,p_z;t).$$

The quantity $f d^3q d^3p$ then represents the probability of finding a particle inside a volume $d\tau = d^3q d^3p$ around the phase space point (x,y,z,p_x,p_y,p_z) at time t. Following Shannon [10], the related information entropy S is given by

$$S(t) = -k_B \int f \ln f \, d\tau, \tag{1}$$

with f the six-dimensional μ-phase space density function. The change of the so-defined entropy, hence the time derivative of Eq. (1), then follows as:

$$\frac{dS}{dt} = -k_B \int (1+\ln f) \frac{\partial f}{\partial t} d\tau. \tag{2}$$

This definition of an entropy does not contain any resolution-dependent features. If we could manage to measure directly the μ-phase space entropy, we would obtain the value of S as defined in Eq. (1) only in the limit of perfect resolution. In contrast, a real measuring device would provide us with a reduced amount of information on the μ-phase space density function. We could expect the measured coarse-grained entropy S_{cg} to be larger than the true entropy S. In any case, the respective value of S_{cg} depends largely on the specific resolution of a measuring device. It is thus not suited for a general purpose analysis. We will therefore use the entropy definition (1) throughout in this article, keeping in mind that it only constitutes an *idealized* entropy with regard to finite resolution measuring devices.

III. LIOUVILLEAN DYNAMICS

It can easily be shown that the total time derivative of the μ-phase space density function f vanishes, i.e., the μ-phase space Liouville theorem applies if the particles do not interact and if the time evolution of their coordinates follows Hamilton's canonical equations. For charged particle beams whose self-fields must be taken into account, Liouville's theorem for the μ-space f remains fulfilled if the self-fields can be treated analogously to the external focusing fields. Explicitly, $df/dt = 0$ leads to

$$\frac{\partial f}{\partial t} = \sum_{i=1}^{3} \left(\frac{\partial f}{\partial p_i} \frac{\partial H}{\partial x_i} - \frac{\partial f}{\partial x_i} \frac{\partial H}{\partial p_i} \right). \tag{3}$$

Inserting Eq. (3) into (2), we obtain, after integration by parts,

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

Here we have made 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. Consequently, all integrated expressions evaluate to zero at the integration boundaries. Summarizing the above result, we may write

$$\frac{df}{dt} = 0 \Rightarrow \frac{dS}{dt} = 0\,, \tag{4}$$

i.e., the entropy change vanishes as long as Liouville's theorem applies for f. Liouville's theorem for the μ-space f does not apply if, for example, particle-particle interactions (''intrabeam scattering'') take place. Thus if the actual ''granularity'' of the charge distribution must be taken into account, we can no longer assume that the ''single-particle'' distribution function f, i.e., the lowest order of the ''Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy'' [11], contains all necessary data on the actual beam.

According to (4), entropy changes are directly related to violations of the μ-phase space Liouville theorem. An increase of entropy just implies an increase of the μ-phase space volume that the beam occupies and hence an absolute degradation of the beam quality. 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. (1). Surely, 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. Nevertheless, this process is not reflected by our definition of the entropy since in the infinite resolution limit a filamentation does not mean any loss of information.

IV. ENTROPY CHANGE ASSOCIATED WITH A MARKOV PROCESS

A precise analysis of effects that are due to the ''granularity'' of the charge distribution requires taking into account the phase space coordinates of *individual* particles. Obviously this kind of problem can never be tackled on the basis of the deterministic approach embodied in the Vlasov equation. On the contrary, a *stochastic* contribution to the net forces acting on a particle must be added. In analogy to the Fokker-Planck description of the Brownian motion of particles, we may model the action of random forces within a beam by a process whose state at time $t+\Delta t$ depends only on its state at time t and *not* on earlier times. Here Δt denotes a characteristic time interval that must be small as compared to the time scale of macroscopic changes of the system. A stochastic process possessing this property is usually referred to as a Markov process. It is easily shown [12] that the equation of motion of such processes is given by the Fokker-Planck equation. The description of particle dynamics including stochastic forces can thus be based on the combined Vlasov-Fokker-Planck equation [1]

$$\frac{\partial f}{\partial t}+\frac{\vec{p}}{m}\cdot\vec{\nabla}_x f+(\vec{F}^{\text{ext}}+q\vec{E}^{\text{sc}})\cdot\vec{\nabla}_p f=\left[\frac{\partial f}{\partial t}\right]_{\text{FP}}, \tag{5}$$

with

$$\left[\frac{\partial f}{\partial t}\right]_{\text{FP}}=-\sum_i \frac{\partial}{\partial p_i}[F_i(\vec{p},t)f] + m^2\sum_{i,j}\frac{\partial^2}{\partial p_i\partial p_j}[D_{ij}(\vec{p},t)f].$$

In this notation, $\vec{F}^{\text{ext}}$ stands for the applied external focusing forces, $q\vec{E}^{\text{sc}}$ for the macroscopic electric space charge forces, $F_i(\vec{p},t)$ for the ''drift vector'' components of the Fokker-Planck equation, and $D_{ij}(\vec{p},t)$ for its ''diffusion tensor'' elements. As shown in the preceding section, the Vlasov terms do not contribute to any entropy production. Therefore, Eq. (2) can be rewritten as

$$\frac{dS}{dt}=-k_B\int(1+\ln f)\left[\frac{\partial f}{\partial t}\right]_{\text{FP}}d\tau. \tag{6}$$

Explicitly this means

$$\frac{dS}{dt}=k_B\int(1+\ln f)\left\{\sum_i\frac{\partial}{\partial p_i}[F_i(\vec{p},t)f] - m^2\sum_{i,j}\frac{\partial^2}{\partial p_i\partial p_j}[D_{ij}(\vec{p},t)f]\right\}d\tau. \tag{7}$$

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

$$\int(1+\ln f)\frac{\partial}{\partial p_i}[F_i f]\,d\tau=\int\frac{\partial F_i}{\partial p_i}f\,d\tau.$$

Again we take advantage of the fact that for real beams the phase space density f as well as all its derivatives vanish at the integration boundaries.

It has been shown by Reiser [13] that the Maxwell-Boltzmann distribution is the only one that provides a steady-state solution of both, the time-independent Vlasov equation and the time-independent Fokker-Planck equation. We conclude that this distribution is best suited for the description of a ''steady-state beam,'' i.e., a beam which has adapted itself to the focusing structure. Since the applied external forces vary along that structure, a charged particle beam can never completely settle down to equilibrium. Therefore, the instantaneous velocity distribution of a real beam must be approximated by a nonisotropic Maxwell-Boltzmann distribution that generalizes the steady-state idealization

$$f=g(x,y,z;t)\exp\left(-\frac{p_x^2}{2mk_BT_x}-\frac{p_y^2}{2mk_BT_y}-\frac{p_z^2}{2mk_BT_z}\right), \tag{8}$$

with $g(x,y,z;t)$ as the self-consistent charge density and the exponential function describing the distribution of the incoherent part of the kinetic particle energy. The coherent part of the kinetic energy of the beam particles—which originates in the ''breathing'' of the beam envelopes—can be eliminated since it does not cause any entropy changes. We may therefore restrict ourselves in Eq. (8) to a principle axes formulation even for the case of a strong focusing and dispersive system.

With the phase space density function (8), the terms of the second sum of Eq. (7) evaluate to

$$m^2\int(1+\ln f)\frac{\partial^2}{\partial p_i\partial p_j}[D_{ij}f]d\tau=-\frac{m}{k_BT_i}\delta_{ij}\int D_{ij}f\,d\tau.$$

In summary, the change of entropy caused by a Markov process can be expressed in terms of the Fokker-Planck coefficients as

$$\frac{dS}{dt}=k_B\sum_{i=1}^{3}\left(\left\langle\frac{\partial F_i}{\partial p_i}\right\rangle+\frac{m}{k_BT_i}\langle D_{ii}\rangle\right), \tag{9}$$

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

V. ORNSTEIN-UHLENBECK PROCESSES

The Fokker-Planck model, as expressed mathematically in Eq. (5), 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 velocity 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 [14]. The latter are defined by the property that its Fokker-Planck equation contains a linear drift coefficient together with a constant diffusion coefficient

$$F_i=-\beta_{f;i}p_i,\quad \beta_{f;i},D_{ii}=\text{const.} \tag{10}$$

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. Therefore Eq. (9) simplifies to

$$\frac{dS}{dt}=k_B\sum_i\left(-\beta_{f;i}+\frac{m}{k_BT_i}D_{ii}\right). \tag{11}$$

Equation (11) forms the basis for establishing a relation between entropy and rms emittance, as will be shown in the next section.

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 being approximately isotropic. Equation (11) then becomes

$$\frac{dS}{dt}=k_B\sum_i\left(-\beta_f+\frac{m}{k_BT_i}D\right).$$

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 diffusion coefficients D_{ii} are related to the friction terms $\beta_{f;i}$ via a fluctuation-dissipation theorem. In the simplest case of an isotropic process, this theorem is embodied in the Einstein relation [6]

$$D=\beta_f\frac{k_BT}{m},$$

wherein $T=\frac{1}{3}\Sigma_i T_i$ stands for the equilibrium temperature. The entropy change due to a temperature balancing process may then be written as

$$\frac{dS}{dt}=k_B\beta_f\sum_i\left(\frac{T}{T_i}-1\right), \tag{12}$$

or, explicitly

$$\frac{dS}{dt}=\frac{1}{3}k_B\beta_f\left[\frac{(T_x-T_y)^2}{T_xT_y}+\frac{(T_x-T_z)^2}{T_xT_z}+\frac{(T_y-T_z)^2}{T_yT_z}\right]. \tag{13}$$

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

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

The total heat exchange dQ/dt vanishes, as is easily seen from Eq. (12)

$$\frac{dQ}{dt}\equiv\sum_i T_i\frac{dS_i}{dt}=k_B\beta_f\sum_i(T-T_i)\equiv 0. \tag{14}$$

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. (13). We conclude that equipartitioning effects occurring within initially thermally unbalanced charged particle beams are always associated with an irreversible degradation of the beam quality as a whole. Furthermore instantaneous temperature differences may exist even if the beam is perfectly matched in all its moments on the average over one focusing period. In beam transport systems with quadrupole focusing, apart from isolated locations, the instantaneous transverse temperatures are always different. Therefore a certain growth rate—depending on the size of the temperature differences—can never be avoided.

The time scale for this process is determined by the frequency β_f. As the result of averaging procedures [12,13], this follows from the global beam parameters as:

$$\beta_f=\frac{16\sqrt{\pi}}{3}nc\left(\frac{q^2}{4\pi\epsilon_0mc^2}\right)^2\left(\frac{mc^2}{2k_BT}\right)^{3/2}\ln\Lambda. \tag{15}$$

In this equation, n stands for the real space average particle density and $\ln\Lambda$ for the Coulomb logarithm.

VI. ENTROPY AND RMS EMITTANCE

A second order moment analysis of the generalized Liouville equation (5) yields the following set of coupled equations of motion [4] for each phase space plane $i=1,2,3$:

$$\frac{d}{dt}\langle x_i^2\rangle-\frac{2}{m}\langle x_ip_i\rangle=0,$$

$$\frac{d}{dt}\langle x_ip_i\rangle-\frac{1}{m}\langle p_i^2\rangle-\langle x_iF_i^{\rm ext}\rangle-q\langle x_iE_i\rangle=\langle x_iF_i\rangle, \tag{16}$$

$$\frac{d}{dt}\langle p_i^2\rangle-2\langle p_iF_i^{\rm ext}\rangle-2q\langle p_iE_i\rangle=2\langle p_iF_i\rangle+2m^2\langle D_{ii}\rangle,$$

with $F_i^{\rm ext}$ the components of the external focusing forces. Again, the angle brackets enclose the respective averages over the phase space density function: $\langle a\rangle=\int af\,d\tau$. Using canonical variables, the rms emittance in the beam system is usually defined as

$$\varepsilon_{i,\rm rms}^2(t)=\langle x_i^2\rangle\langle p_i^2\rangle-\langle x_ip_i\rangle^2. \tag{17}$$

Since no other definitions of emittance are used throughout this article, we will skip the index ''rms'' in the following. On calculating the time derivative of ε_i^2(t), we readily obtain

$$\begin{aligned}\frac{d}{dt}\varepsilon_i^2(t)=&2[\langle x_i^2\rangle\langle p_iF_i^{\rm ext}\rangle-\langle x_ip_i\rangle\langle x_iF_i^{\rm ext}\rangle]+2q[\langle x_i^2\rangle\langle p_iE_i\rangle\\&-\langle x_ip_i\rangle\langle x_iE_i\rangle]+2[\langle x_i^2\rangle\langle p_iF_i\rangle-\langle x_ip_i\rangle\langle x_iF_i\rangle]\\&+2m^2\langle x_i^2\rangle\langle D_{ii}\rangle.\end{aligned} \tag{18}$$

The terms containing the external field components cancel if these fields can be regarded as linear

$$F_i^{\rm ext}\propto x_i\Leftrightarrow\langle x_i^2\rangle\langle p_iF_i^{\rm ext}\rangle\equiv\langle x_ip_i\rangle\langle x_iF_i^{\rm ext}\rangle. \tag{19}$$

The so-called ''excess field energy,'' namely, the difference between the field energy W of an *arbitrary* charge distribution and the field energy $W^{\rm u}$ of a *uniform* charge distribution of the same rms size, is given by [9,15]

$$\frac{d}{dt}(W-W^u)=-\frac{Nq}{m}\sum_i\left(\langle p_iE_i\rangle-\frac{\langle x_ip_i\rangle}{\langle x_i^2\rangle}\langle x_iE_i\rangle\right). \tag{20}$$

We observe that the terms of the sum in Eq. (20) exactly correspond to the moments involving the electric self-fields E_i in (18).

Assuming again that the non-Liouvillean process can be approximated by an Ornstein-Uhlenbeck process, we may simplify the Fokker-Planck coefficients according to Eq. (10). Together with Eqs. (19) and (20), the equation of motion for the rms emittance (18) can be rewritten as

$$\frac{1}{\langle x_i^2\rangle}\frac{d}{dt}\varepsilon_i^2(t)=-2\beta_{f;i}\frac{\varepsilon_i^2(t)}{\langle x_i^2\rangle}+2m^2D_{ii}-\frac{2m}{N}\frac{d}{dt}(W_i-W_i^{\mathrm{u}}), \tag{21}$$

with $W_i-W_i^{\mathrm{u}}$ denoting formally the ith component of the sum (20).

The global ''temperature'' T_i of the ith degree of freedom of a charged particle beam can be expressed in terms of second order beam moments

$$k_BT_i=\frac{1}{m}\frac{\varepsilon_i^2(t)}{\langle x_i^2\rangle}, \tag{22}$$

provided that the projections of the phase space density function f onto two-dimensional subspaces (x_i,p_i) are homogeneously populated. To a good approximation, this expression can be applied to arbitrary phase space density functions f since the respective error always vanishes at the extremities of the beam envelopes [4].

With the help of this approximation, the temperature T_i contained in the equation for change of entropy (11) can be replaced by the corresponding beam moments

$$\frac{dS}{dt}=\sum_i\frac{dS_i}{dt},\quad \frac{dS_i}{dt}=k_B\left(-\beta_{f;i}+m^2\frac{\langle x_i^2\rangle}{\varepsilon_i^2(t)}D_{ii}\right). \tag{23}$$

Inserting Eq. (23) into (21), we obtain an equation relating emittance, entropy and excess field energy

$$\frac{1}{\langle x_i^2\rangle}\frac{d}{dt}\varepsilon_i^2(t)=\frac{2\,\varepsilon_i^2(t)dS_i}{k_B\langle x_i^2\rangle\,dt}-\frac{2m\,d}{N\,dt}(W_i-W_i^{\mathrm{u}}). \tag{24}$$

As the last step, the summation over i must be performed

$$\sum_i\frac{1}{\langle x_i^2\rangle}\frac{d}{dt}\varepsilon_i^2(t)+\frac{2m}{N}\frac{d}{dt}(W-W^u)$$
$$=2m\sum_i T_i\frac{dS_i}{dt}=0\quad\text{for isotropic FP coefficients.} \tag{25}$$

As stated before in Eq. (14), the right hand side of (25) sums up to zero under the precondition of isotropic Fokker-Planck coefficients. Equation (25) then constitutes the known relationship between the changes of the rms emittances and the change of the excess field energy, first derived by Wangler [9,16,15] 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 approximately be described by isotropic Fokker-Planck coefficients.

Multiplying Eq. (24) with $\langle x_i^2\rangle/2\varepsilon_i^2(t)$ leads to the equivalent form

$$\frac{1}{k_B}\frac{dS_i}{dt}=\frac{d}{dt}\ln\varepsilon_i(t)+\frac{m}{N}\frac{\langle x_i^2\rangle}{\varepsilon_i^2(t)}\frac{d}{dt}(W_i-W_i^{\mathrm{u}})\,. \tag{26}$$

Summing now Eq. (26) over i, the time derivative of the entropy function $S(t)$ becomes

$$\frac{1}{k_B}\frac{dS}{dt}=\frac{d}{dt}\ln\varepsilon_x(t)\varepsilon_y(t)\varepsilon_z(t)+\frac{m}{N}\sum_i\frac{\langle x_i^2\rangle}{\varepsilon_i^2(t)}\frac{d(W_i-W_i^u)}{dt}$$
$$=\frac{d}{dt}\ln\varepsilon_x(t)\varepsilon_y(t)\varepsilon_z(t)-q$$
$$\times\sum_i\frac{\langle x_i^2\rangle\langle p_iE_i\rangle-\langle x_ip_i\rangle\langle x_iE_i\rangle}{\varepsilon_i^2(t)}. \tag{27}$$

This equation constitutes a general relation between entropy change, the change of the rms emittances, and the temperature weighted change of the excess field energy for the realm of ion optics. It thus confirms the heuristic approach presented earlier by Lawson, Lapostolle, and Gluckstern [17], who showed the close relation between the entropy and beam emittance.

With the heat differential dQ_i defined as

$$dQ_i=k_BT_i d\ln\varepsilon_i+\frac{1}{N}d(W_i-W_i^u),$$

Eq. (27) reads

$$dS=\sum_i\frac{dQ_i}{T_i},$$

using the temperature definition of Eq. (22). For the special case of isotopic Fokker-Planck coefficients, the emittance to the excess field energy relation (25) then takes on the simple form

$$\sum_i dQ_i=0.$$

We note that Eq. (24) as well as Eq. (26) do not contain any Fokker-Planck coefficients—although they are derived on the basis of the Fokker-Planck approach (5). Recalling Eq. (21), we see that the Fokker-Planck related moments exactly agree with those appearing in Eq. (9), provided that we restrict ourselves to Ornstein-Uhlenbeck processes, and the global temperature definition (22). Under these preconditions, the insertion of Eq. (23) into Eq. (21) 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. (24) and (26) just by allowing for changes of the entropy (1), and *not* by eliminating entropy changes dS_i *a priori*, as it is done in a Vlasov approach.

In the course of this derivation, the temperatures T_i, as defined in Eq. (22), are understood as global temperatures pertaining to the ith degree of freedom. Implicitly, we thus assumed that no heat is transferred within each degree of freedom. In other words we only treat cases where the beam has already adapted itself to the focusing lattice, i.e., cases where no transient effects are observed. This condition is not necessarily fulfilled. It has been shown numerically by various authors (cf. [7,18,19], for example) that a redistribution of the populated phase space—occurring if a beam is launched with a non-self-consistent phase space filling—also constitutes an irreversible process. These effects are not covered by our approach since for non-self-consistent phase

space densities, a transfer of heat also takes place within each degree of freedom. A global temperature description is not sufficient under these circumstances. On the contrary, a local, i.e., spatially dependent ''temperature'' definition must be used instead.

VII. DISCUSSION

A. 1D beam model

For the sake of mathematical simplicity, the sheet beam model is sometimes applied, since it allows analytical solutions for cases where more realistic models depend on numerical methods. Of course, the one-dimensional beam model is oversimplified in the sense of not allowing heat transfer to other degrees of freedom. With regard to the derivations of the last section, this means that no summation over i must be performed. In other words, because of this model, Eqs. (25) and (27) are equivalent

$$\frac{1}{k_B}\frac{dS}{dt}=\frac{\langle x^2\rangle}{2\varepsilon_x^2(t)}\left[\frac{1}{\langle x^2\rangle}\frac{d}{dt}\varepsilon_x^2(t)+\frac{2m}{N}\frac{d}{dt}(W-W^{\mathrm{u}})\right]\equiv 0.$$

Consequently, all solutions of the Vlasov-Fokker-Planck equation (5) are reversible if the initial phase space density function is intrinsically matched. This behavior of sheet beams has been described and numerically simulated earlier by Anderson [19], who showed the existence of strictly reversible changes of the rms emittance.

B. 2D beam model

The two-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. With the equilibrium temperature $T=\frac{1}{2}(T_x+T_y)$ for the 2D beam model, Eq. (12) for the entropy change near thermodynamic equilibrium can be rewritten as

$$\frac{dS}{dt}=\frac{1}{2}k_B\beta_f\frac{(T_x-T_y)^2}{T_xT_y}. \tag{28}$$

Beam transport without an increase of entropy (i.e., reversible beam transformations) are thus possible if either

(1) $\beta_f\equiv 0$, which means that no non-Liouvillean effects are present, or if

(2) $T_x\equiv T_y$, i.e., the beam stays round throughout its propagation.

The first case just describes the pure Vlasov approach, which is, by our definition of the entropy in Eq. (1), always associated with a vanishing entropy growth, as already stated in Sec. III.

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 2D beam model if we transform a matched beam through a continuous or interrupted solenoid channel.

We note that with regard to intrabeam scattering effects, the heat exchange with the longitudinal degree of freedom cannot be neglected. In other words, the 2D beam model is not adequate for the estimation of emittance growth rates due to intrabeam scattering. This topic will be discussed in the next subsection.

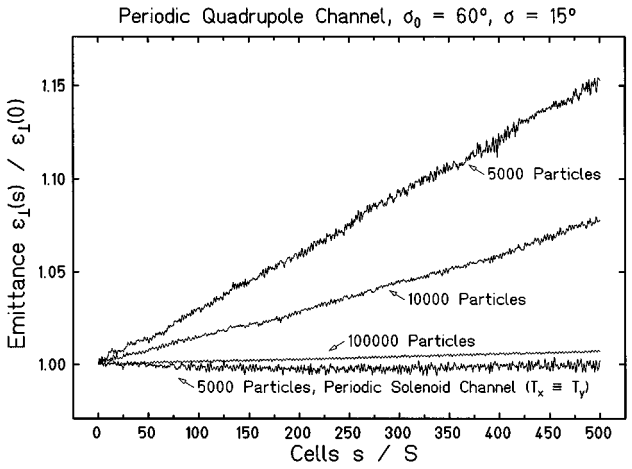

FIG. 1. Emittance growth factors versus number of cells obtained by 2D particle-in-cell simulations of beam transport channels at $\sigma_0=60°$, $\sigma=15°$. s denotes the propagation distance of the beam, S denotes the period length. The upper three curves display the results of quadrupole channel simulations with different numbers of simulation particles. For comparison, the lowest curve shows the emittance growth factors of a periodic solenoid channel simulation.

Nevertheless, Eq. (28) can help us to interpret results of computer simulations that are based on the 2D beam model. The upper three curves in Fig. 1 show the evolution of the rms-emittance growth factors along a quadrupole channel as they are obtained for different numbers of macroparticles used in the simulation, while keeping all other simulation parameters unchanged. In all cases, the beam is launched with a self-consistent water-bag distribution [20,21,15] for the initial phase space population. The external focusing has been approximated by strictly linear forces and the hard edge lens model. The space charge fields have been determined using a fast x,y Poisson solver with 128 by 128 mesh nodes. Under these circumstances only the space charge fields can contribute to a growth of the rms emittances. Since the growth rates obtained as well as the amplitude of the emittance fluctuations are approximately inversely proportional to the number of macroparticles used in the simulation, it is obviously the inaccuracies in calculating these fields that are responsible for the growth of the rms emittance. With regard to Eq. (28), we conclude that these inaccuracies induce a positive ''simulation friction coefficient'' β_f^{sim}, which is to first order inversely proportional to the number of simulation particles.

Using Eq. (28) to explain simulation results means, after all, to use the Fokker-Planck equation (5) as the basis for the description of purely numerical noise phenomena. The validity of this approach becomes obvious if we recall that the gradual loss of information due to simplifications and round-off errors itself constitutes a Markov process which in turn can be modeled by the Fokker-Planck equation.

This statement is confirmed by the simulation results displayed in the lower curve of Fig. 1. It shows the evolution of the rms-emittance growth factors during the propagation of a matched beam through a periodic solenoid channel. Since the beam stays round along the entire channel, no transverse temperature gradient exists, hence no entropy change is expected according to Eq. (28). We observe that the emittance fluctuations are similar in amplitude to those in the quadru-

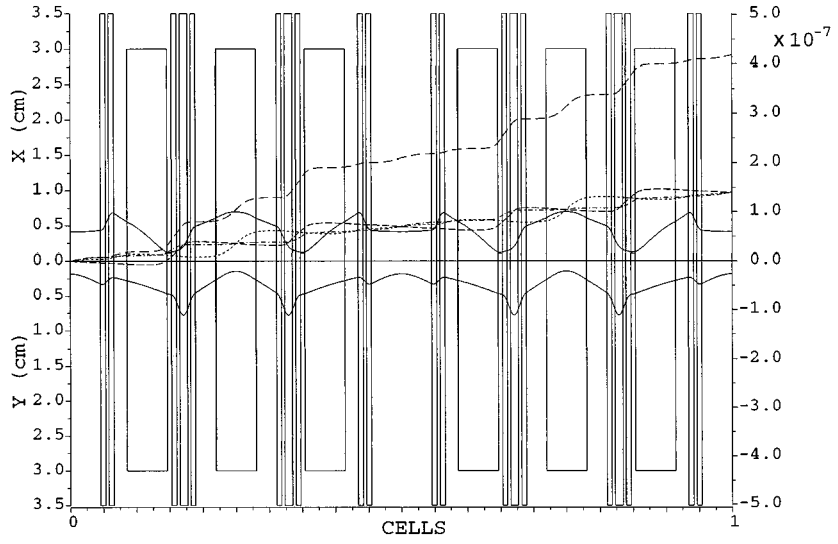

FIG. 2. Envelopes (solid lines), emittance growth functions ($\varepsilon_x/\varepsilon_{x;0}-1$: dotted line, $\varepsilon_y/\varepsilon_{y;0}-1$: dashed line, $\varepsilon_z/\varepsilon_{z;0}-1$: dashed-dotted line), and entropy function $(S-S_0)/k_B$ (upper dashed line) of a thermally matched beam passing through one turn of the GSI experimental storage ring (ESR) at $Q_h=2.31$ and $Q_v=2.25$. The scale on the right hand side applies to the dimensionless emittance and entropy growth functions.

pole channel simulation performed with the same number of macroparticles. This means that in both cases the fluctuating part of the self-fields impose a similar ''simulation friction coefficient'' $\beta_f^{\rm sim}$. Yet, due to the lack of temperature differences, these fluctuations do *not* produce an overall increase of the rms emittance.

C. 3D beam

We first consider the hypothetical case of a beam that is thermally balanced in all three dimensions, i.e., $T=T_x=T_y=T_z$. As is easily seen, Eqs. (25) and (27) are again equivalent in this case, which in turn means that the entropy remains constant. If we imagine this beam is ''breathing'' isotropically in all three directions, a completely reversible exchange between the rms emittances and the excess field energy (20) would take place. In this sense we may state that

(1) a change of the rms emittance due to a change of the excess field energy is a *reversible* process, whereas

(2) a change of the rms emittance due to a flow of heat is always an *irreversible* process.

In real beam guiding systems, we must always cope with a specific amount of temperature anisotropy and hence always deal with a positive growth rate of the entropy. The elementary mechanism responsible for the transfer of incoherent kinetic energy from one degree of freedom to another is constituted by the effect of Coulomb scattering of individual beam particles. This effect forms the basis for deriving Eq. (15). We may therefore use it in order to estimate the time scale for heat flow effects, or, equivalently, the scattering induced irreversible emittance growth rates. In order to gain a better physical insight, the frequency β_f can be expressed alternatively as

$$\beta_f=\sqrt{\frac{2}{\pi}}(t_{\rm scattering})^{-1}\Gamma^2\ln\Lambda,$$

with $t_{\rm scattering}^{-1}$ denoting the number of scattering events within the beam per time (''scattering rate''), and Γ the dimensionless coupling constant of the beam plasma.

If we neglect the (reversible) changes of the rms emittance due to changes of excess field energy, on the basis of Eqs. (16) we may easily establish a closed coupled set of generalized envelope and temperature change equations [22,4] which can be directly integrated. The results of an integration of this set of equations based on the geometry of the Gesellschaft für Schwerionenforschung (GSI) experimental storage ring (ESR) are plotted in Fig. 2. It includes the dispersion function [23] for the particular tuning of the ring. The ratios of the initial emittances have been optimized to yield the same growth rates in all three dimensions. The upper dashed curve thus displays the minimum entropy growth $(S-S_0)/k_B$ during one turn.

Integrating Eq. (13) we find

$$\frac{1}{k_B}[S(t)-S_0]=\frac{1}{3}\beta_f t[I_{xy}(t)+I_{xz}(t)+I_{yz}(t)],$$

with

$$I_{xy}(t)=\frac{1}{t}\int_{t_0}^{t}\frac{[T_x(t')-T_y(t')]^2}{T_xT_y}dt',$$

and with $I_{xz}(t)$ and $I_{yz}(t)$ to be defined likewise. If the global beam data, thus β_f, is given, we can only reduce the entropy production by minimizing the dimensionless sum

$$I(t_1)=I_{xy}(t_1)+I_{xz}(t_1)+I_{yz}(t_1),$$

where t_1 denotes the time the beam centroid needs to propagate over one focusing period. For a given structure, this implies minimizing the average temperature gradients and hence perfectly matching the beam to the guiding structure in all three dimensions. In our example (Fig. 2), simulating the transformation of a coasting beam through one turn of the ESR—this has been performed by rms matching the transverse beam parameters while at the same time adjusting the initial emittance and momentum spread ratios.

If we are in the design phase of an ion optical system, we may include minimizing of $I(t_1)$ as part of the optimization

of the structure under consideration. This is just an alternative formulation of Reiser's suggestion of a thermodynamic accelerator design [24].

VIII. CONCLUSIONS

We have used a resolution-independent entropy that follows directly from the six-dimensional μ-phase space density function f. This entropy possesses the property of remaining constant as long as Liouville's theorem applies for f. Since in reality as well as in computer simulations of charged particle beams this is not true in a strict sense, we always have to cope with a certain rate of dilution of the μ-phase space density and hence always accept some increase of entropy. For the estimation of this growth, a new equation has been derived on the basis of the Fokker-Planck approach. It relates the change of entropy to the joint changes of the rms emittance and the temperature weighted excess field energy. From this equation, we can conclude that the exchange of rms emittance and excess field energy may be performed without a change of entropy and hence in a reversible manner. In contrast to this, it has been shown that all heat transfers within the beam—feeding thermal energy from one degree of freedom to another—are always associated with an increase of beam entropy and thus always lead to an irreversible degradation of beam quality.

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