

GENERAL PRINCIPLES OF KINETICS

The first detailed approach to the kinetic description of many particle systems appeared in the famous works of Boltzmann (1872, 1895, 1898). The main idea of the derivation of a kinetic equation is to describe a complex system dynamics using a reduced number of variables. For example, a complete description of a dynamical system can be done with a Liouville equation:

$$\frac{\partial F}{\partial t} + \dot{\boldsymbol{\vartheta}} \cdot \frac{\partial F}{\partial \boldsymbol{\vartheta}} + \dot{\mathbf{I}} \cdot \frac{\partial F}{\partial \mathbf{I}} = 0, \quad (14.1)$$

where $\mathbf{I} \in \mathbb{R}^N$, $\boldsymbol{\vartheta} \in \mathbb{R}^N$, $F = F(\mathbf{I}, \boldsymbol{\vartheta}, t)$ is the density distribution function in phase space, and $(\mathbf{I}, \boldsymbol{\vartheta})$ satisfy the Hamiltonian equations. There are two typical reductions of variables:

- (i) averaging over fast variables, phase $\boldsymbol{\vartheta}$, and the corresponding transition

$$F = F(\mathbf{I}, \boldsymbol{\vartheta}, t) \rightarrow F(\mathbf{I}, t) \quad (14.2)$$

- (ii) transition from N -degrees of freedom to one degree of freedom

$$F(\mathbf{I}, t) \rightarrow F(I, t), \quad I \in \mathbb{R}. \quad (14.3)$$

All approaches and methods exploit a randomness of the dynamics in explicit or implicit form and due to the fact all kinetic equations acquire a remarkable feature, *irreversibility*, and they satisfy the so-called H -theorem that also has been discovered by Boltzmann (*Note 14.1*).

Dynamical chaos gives rise to a new vision of the basic principles of kinetics. The main feature of a new wave in kinetic theories is that the random element of the dynamics can be found directly from the Hamiltonian equation of motion, in contrast to introducing randomness as an assumption. New models of the kinetic theory are sometimes very different from the previously known types of kinetic equations, and this will be the subject of the following chapters (*Note 14.2*).

14.1 Time scales

All approximate methods of the derivation of kinetics require a differentiation of time-scales. Here are presented the most typical ones.

The collision time τ_{coll} characterizes the duration of a 'collision' of a particle with external object or field. Typically this time shows how long a perturbation

acts on the particle. As a result of this action, there is a change of variables $\Delta I, \Delta \vartheta$. The value Δt_{coll} is the time interval between two adjacent collisions. A 'good' situation is when

$$\tau_{\text{coll}} \ll \Delta t_{\text{coll}}, \quad (14.4)$$

which means that particle dynamics can be considered as unperturbed, that is, free, between any two adjacent collisions. The introduction of the notion of 'collision time' is meaningful only in the case (14.4). It also permits to introduce a map

$$(I_{n+1}, \vartheta_{n+1}) = \hat{T}_n(I_n, \vartheta_n) \quad (14.5)$$

or in a more specific form

$$\begin{aligned} I_{n+1} &= I_n + f_1(I_n, \vartheta_n), \\ \vartheta_{n+1} &= \vartheta_n + \omega_n \Delta t_n + f_2(I_n, T_n), \end{aligned} \quad (14.6)$$

where f_1, f_2 are some functions related to the perturbation, ω_n is frequency, and Δt_n is a time interval between n -th and $(n+1)$ -th collisions. For example, in the standard map

$$f_2 = f_1 = K \sin \vartheta_n, \quad \Delta t_n = \text{const} = T, \quad \omega_n = \frac{I_n}{T} \quad (14.7)$$

and the condition (14.4) is automatically valid since $\tau_{\text{coll}} = 0$.

As a result of perturbation, one can expect the occurrence of chaotic dynamics that has at least two time-scales. The first one is a time τ_c of the decay of phase correlations. In the good mixing or Anosov-type systems it is of the order

$$\tau_c \sim \frac{\Delta t}{h} \sim \frac{\Delta t}{\sigma}, \quad (14.8)$$

where h is KS-entropy and σ is a dimensionless Lyapunov exponent. For some cases of the standard map and $K \gg 1$

$$\tau_c = \frac{2T}{\ln K}, \quad (14.9)$$

that is, less than a time $\Delta t = T$ between collisions. The second time, due to chaos, describes a slow evolution of the action variable I_n . Typically, this time τ_d satisfies the condition

$$\tau_d \gg \tau_c \quad (14.10)$$

and is known as *diffusion time*.

How these time scales work will be demonstrated using some simple examples, but our main emphasis is that for typical Hamiltonian dynamics the described

scheme is very insufficient due to the presence of singular zones, dynamical traps, etc. Just these deviations from regular (or normal) kinetics make it necessary to extend the class of possible equations to the so-called fractal kinetic equations (*Note 14.3*).

14.2 Fokker-Planck-Kolmogorov (FPK) equation

The FPK equation was obtained by Fokker (1914), Smolukhowski (1915), Einstein (1905), and Planck (1917). Landau (1937) and Kolmogorov (1938) derived the kinetic equation using a special scheme and conditions that are important for understanding some basic principles of kinetics (*Note 14.4*). Let $W(x, t; x', t')$ be a probability density of having a particle at the position x at time t if the particle was at the position x' at time $t' \leq t$. A chain equation of the Markov-type process can be written for $W(x, t; x', t')$:

$$W(x_3, t_3; x_1, t_1) = \int dx_2 W(x_3, t_3; x_2, t_2) W(x_2, t_2; x_1, t_1), \quad (14.11)$$

which has a simple meaning that the transition $(x_1, t_1) \rightarrow (x_3, t_3)$ can go through all possible states (x_2, t_2) .

A typical assumption for W is its time uniformity, i.e.:

$$W(x, t; x', t') = W(x, x'; t - t'). \quad (14.12)$$

Consider the evolution of $W(x, x'; t - t')$ during an infinitesimal time $\Delta t = t' - t$ and use the expansion

$$W(x, x_0; t + \Delta t) = W(x, x_0; t) + \frac{\partial W(x, x_0; t)}{\partial t} \Delta t + \dots \quad (14.13)$$

Equation (14.13) is valid providing the limit:

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \{W(x, x_0; t + \Delta t) - W(x, x_0; t)\} = \frac{\partial W(x, x_0; t)}{\partial t} \quad (14.14)$$

has a sense. The existence of the limit (14.14) for $\Delta t \rightarrow 0$ imposes specific physical constraints that will be discussed in Section 14.4.

Let us now introduce a new notation:

$$P(x, t) \equiv W(x, x_0; t), \quad (14.15)$$

where the initial coordinate x_0 is omitted. With the help of Eqs. (14.11)–(14.13), we can transform (14.14) into:

$$\frac{\partial P(x, t)}{\partial t} = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int dy W(x, y; \Delta t) P(y, t) - P(x, t) \right\}. \quad (14.16)$$

The first important feature in the derivation of the kinetic equation is the introduction of two distribution functions $P(x, t)$ and $W(x, y; \Delta t)$ instead of the one $W(x, t; x', t')$. The function $P(x, t)$ will be used for $t \rightarrow \infty$ or, more accurately, for t which satisfies the condition

$$t \gg \tau_{\text{coll}}, \quad (14.17)$$

where τ_{coll} is not defined yet. In this situation $W(x, x_0; t)$ does not depend on the initial condition x_0 and this explains the notation (14.15). Contrary to $P(x, t)$, $W(x, y; \Delta t)$ defines the transition during very short time $\Delta t \rightarrow 0$. For $\Delta t = 0$ it should be no transition at all if the velocity is finite, i.e.:

$$\lim_{\Delta t \rightarrow 0} W(x, y; \Delta t) = \delta(x - y). \quad (14.18)$$

Following this restriction we can use the expansion over δ -function and its derivatives (Zaslavsky 1994a; Zaslavsky 1994b), i.e.:

$$W(x, y; \Delta t) = \delta(x - y) + A(y; \Delta t)\delta'(x - y) + \frac{1}{2}B(y; \Delta t)\delta''(x - y), \quad (14.19)$$

where $A(y; \Delta t)$ and $B(y; \Delta t)$ are some functions. The prime denotes a derivative with respect to the argument, and we consider the expansion up to the second order only.

Distribution $W(x, y; \Delta t)$ is called *transfer probability* and it satisfies two normalization conditions:

$$\int W(x, y; \Delta t) dx = 1 \quad (14.20)$$

and

$$\int W(x, y; \Delta t) dy = 1. \quad (14.21)$$

The coefficients $A(x; \Delta t)$ and $B(x; \Delta t)$ have a fairly simple meaning. They can be expressed as moments of $W(x, y; \Delta t)$:

$$\begin{aligned} A(y; \Delta t) &= \int dx (y - x) W(x, y; \Delta t) \equiv \langle\langle \Delta y \rangle\rangle, \\ B(y; \Delta t) &= \int dx (y - x)^2 W(x, y; \Delta t) \equiv \langle\langle (\Delta y)^2 \rangle\rangle. \end{aligned} \quad (14.22)$$

In a similar way, coefficients for the higher orders of the expansion of $W(x, y; \Delta t)$ can be expressed through the higher moments of W .

Integration of (14.19) over x does not provide any additional information due to (14.20), but integrating over y and using (14.21) gives:

$$A(y; \Delta t) = \frac{1}{2} \frac{\partial B(y; \Delta t)}{\partial y} \quad (14.23)$$

or applying the notations (14.22),

$$\langle\langle\Delta y\rangle\rangle = \frac{1}{2} \frac{\partial}{\partial y} \langle\langle(\Delta y)^2\rangle\rangle. \quad (14.24)$$

Expressions (14.23) and (14.24) were first obtained in Landau (1937) as a result of the *microscopic reversibility*, or detailed balance principle. In Landau (1937), dynamical Hamiltonian equations were used for (14.24), while here we use the expansion (14.19) and 'reversible' normalization (14.21). The final step is an assumption that we name the following existing limits *Kolmogorov conditions*:

$$\begin{aligned} \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \langle\langle\Delta x\rangle\rangle &\equiv \mathcal{A}(x), \\ \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \langle\langle(\Delta x)^2\rangle\rangle &\equiv \mathcal{B}(x), \\ \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \langle\langle(\Delta x)^m\rangle\rangle &= 0, \quad (m > 2). \end{aligned} \quad (14.25)$$

It is due to the Kolmogorov conditions that irreversibility appears at the final equation. Now it is just formal steps. Substituting (14.19), (14.22), and (14.24) into (14.16) gives

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial}{\partial x} (\mathcal{A}P(x, t)) + \frac{1}{2} \frac{\partial^2}{\partial x^2} (\mathcal{B}P(x, t)), \quad (14.26)$$

which is the equation derived by Kolmogorov and which is called the Fokker-Planck-Kolmogorov (FPK) equation. It is a diffusion-type equation and it is irreversible. After using the relations (14.23) and (14.24) we get the diffusion equation (14.26) in the final form:

$$\frac{\partial P(x, t)}{\partial t} = \frac{1}{2} \frac{\partial}{\partial x} \mathcal{D} \frac{\partial P(x, t)}{\partial x} \quad (14.27)$$

with a *diffusion coefficient*

$$\mathcal{D} = \mathcal{B} = \lim_{\Delta t \rightarrow 0} \frac{\langle\langle(\Delta x)^2\rangle\rangle}{\Delta t}. \quad (14.28)$$

Equation (14.27) has a divergent form that corresponds to the conservation law of the number of particles:

$$\frac{\partial P}{\partial t} = \frac{\partial J}{\partial x} \quad (14.29)$$

with the particle flux

$$J = \frac{1}{2} \mathcal{D} \frac{\partial P}{\partial x}. \quad (14.30)$$

In the following section we will see how a similar scheme can be applied to derive the fractional kinetic equation.

An additional condition follows from (14.24) and notations (14.25) and (14.28)

$$\mathcal{A}(x) = \frac{1}{2} \frac{\partial \mathcal{B}(x)}{\partial x} = \frac{1}{2} \frac{\partial \mathcal{D}}{\partial x}, \quad (14.31)$$

which explains a physical meaning of $\mathcal{A}(x)$ as a convective part of the particle flux. This part of the flux and $\mathcal{A}(x)$ are zero if $\mathcal{D} = \text{const}$ (*Note 14.5*).

14.3 Detailed balance principle

The divergent form (14.27) of the FPK equation is a particular case of (14.26). This form appears due to some symmetry of the moments that follows from (14.23) or (14.24). In its turn, (14.23) is a result of the expansion (14.19) with symmetry conditions (14.20) and (14.21) for the transitional probability. Such condition of symmetry is known as the *detailed balance principle*, and its connection to the divergent form of the kinetic equation was shown by Landau (1937). Landau also has shown in the same paper a simple way to derive (14.24) based on the uniformity of the phase distribution.

Let the Hamiltonian of a system be $H = H(I, \vartheta; t)$ and let us calculate a change of action I during a small time interval Δt up to the terms of the order $(\Delta t)^2$. It follows:

$$\begin{aligned} \Delta I &= I(t + \Delta t) - I(t) = \dot{I} \Delta t + \frac{1}{2} \ddot{I} (\Delta t)^2 \\ &= -\frac{\partial H}{\partial \vartheta} \Delta t - \frac{1}{2} \left\{ \frac{\partial}{\partial \vartheta} \frac{\partial H}{\partial t} + \frac{\partial^2 H}{\partial \vartheta^2} \frac{\partial H}{\partial I} - \frac{\partial^2 H}{\partial I \partial \vartheta} \frac{\partial H}{\partial \vartheta} \right\} (\Delta t)^2, \end{aligned} \quad (14.32)$$

where the Hamiltonian equations

$$\dot{I} = -\frac{\partial H}{\partial \vartheta}, \quad \dot{\vartheta} = \frac{\partial H}{\partial I}, \quad (14.33)$$

have been used and the operator has been applied

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \dot{I} \frac{\partial}{\partial I} + \dot{\vartheta} \frac{\partial}{\partial \vartheta}. \quad (14.34)$$

Finally, (14.32) transfers into

$$\Delta I = -\frac{\partial H}{\partial \vartheta} \Delta t - \frac{1}{2} \frac{\partial}{\partial \vartheta} \left[\frac{\partial H}{\partial t} - \dot{I} \dot{\vartheta} \right] (\Delta t)^2 + \frac{1}{2} \frac{\partial}{\partial I} (\dot{I})^2 (\Delta t)^2. \quad (14.35)$$

We are interested in the coarse-grained, that is, phase averaged, observables. The phase averaging means

$$\langle\langle \dots \rangle\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\vartheta \dots \quad (14.36)$$

that is, any expression that can be presented as ϑ -derivative of some function vanishes after applying (14.36). Thus, up to $(\Delta t)^2$,

$$\begin{aligned} \langle\langle \Delta I \rangle\rangle &= \frac{1}{2} \frac{\partial}{\partial I} \langle\langle \dot{I}^2 \rangle\rangle (\Delta t)^2, \\ \langle\langle (\Delta I)^2 \rangle\rangle &= \langle\langle \dot{I}^2 \rangle\rangle (\Delta t)^2. \end{aligned} \quad (14.37)$$

It follows from (14.15) that

$$\langle\langle \Delta I \rangle\rangle = \frac{1}{2} \frac{\partial}{\partial I} \langle\langle (\Delta I)^2 \rangle\rangle \quad (14.38)$$

be known as a consequence of the *detailed balance* principle, that is, that the probabilities of some transition from a state A to B are the same as for the transition from B to A . The expression (14.38) is similar to the expression (14.24) derived directly from the symmetry of definitions (14.22).

Here we have also to comment that in the proposed qualitative derivation of (14.38) phase averaging that leads to (14.38) is not supported by any microscopic consideration and the way to do it is fairly lengthy. It is also important to mention that $\langle\langle \Delta I \rangle\rangle$ and $\langle\langle (\Delta I)^2 \rangle\rangle$ are of the same order of magnitude.

14.4 Solutions and normal transport

There are numerous sources related to the solutions of the FPK equation (14.27) for different initial and boundary conditions (see for example Weiss (1994); Risken (1989)). Our goal here is just to mention a few simple properties of the FPK equation which are important for the future.

Let us simplify the case considering $\mathcal{D} = \text{const}$, $x \in (-\infty, \infty)$, and the initial condition for a particle to be at $x = 0$. Then

$$P(x, t) = (2\pi \mathcal{D}t)^{-1/2} \exp\left(-\frac{x^2}{2\mathcal{D}t}\right), \quad (14.39)$$

known as a Gaussian distribution. Its odd moments are zero, the second moment is

$$\langle x^2 \rangle = \mathcal{D}t \quad (14.40)$$

and the higher moments are

$$\langle x^{2m} \rangle = \mathcal{D}_m t^m, \quad (m = 1, 2, \dots), \quad (14.41)$$

where $\mathcal{D}_{m=1} = \mathcal{D}$ and $\mathcal{D}_{m>1}$ can be easily expressed through \mathcal{D} but they do not depend on t . (See Problems 14.1–14.3.) There are two properties that we will refer to in the following section: all moments of $P(x, t)$ are finite, as a result of the exponential decay of P for $x \rightarrow \infty$, and the distribution $P(x, t)$ is invariant under the renormalization

$$\hat{R}(a) : x' = ax, \quad t' = a^2 t \quad (14.42)$$

with arbitrary a , that is, the renormalization group $\hat{R}(a)$ is continuous. Evolution of moments $\langle x^m \rangle$ with time will be called *transport*. Dependence (14.40) and (14.41) will be called *normal transport*.

Another type of the distribution function is the so-called moving Gaussian packet

$$P(x, t) = (2\pi\mathcal{D}t)^{-1/2} \exp \left[-\frac{(x - ct)^2}{2\mathcal{D}t} \right] \quad (14.43)$$

with a velocity c . The distribution (14.43) satisfies the equation

$$\frac{\partial P}{\partial t} + c \frac{\partial P}{\partial x} = \frac{1}{2} \mathcal{D} \frac{\partial^2 P}{\partial x^2} \quad (14.44)$$

for which the condition (14.23) or (14.31) fails. They can be restored if we consider the moments $\langle (x - ct)^m \rangle$. It follows from (14.43) that

$$\langle x \rangle = ct \quad (14.45)$$

and

$$\langle (x - \langle x \rangle)^2 \rangle = \mathcal{D}t \quad (14.46)$$

similarly to (14.40).

14.5 Growth of entropy

Consider the magnitude

$$\mathcal{S}_B = -\langle \ln P(x, t) \rangle = -\int_{-\infty}^{\infty} dx P(x, t) \ln P(x, t) \quad (14.47)$$

known as Boltzmann's entropy, and calculate its time evolution

$$\dot{\mathcal{S}}_B = -\frac{d}{dt} \langle \ln P(x, t) \rangle = -\int_{-\infty}^{\infty} dx \frac{\partial P(x, t)}{\partial t} - \int_{-\infty}^{\infty} dx \frac{\partial P(x, t)}{\partial t} \ln P(x, t). \quad (14.48)$$

The first term in the right-hand side is zero due to the normalization condition

$$\int_{-\infty}^{\infty} dx \frac{\partial P(x, t)}{\partial t} = \frac{d}{dt} \int_{-\infty}^{\infty} dx P(x, t) = 0. \quad (14.49)$$

The second term in (14.48) can be modified by using (14.27):

$$\begin{aligned} \int_{-\infty}^{\infty} dx \frac{\partial P(x, t)}{\partial t} \ln P(x, t) &= \frac{1}{2} \int_{-\infty}^{\infty} dx \ln P(x, t) \frac{\partial}{\partial x} \left\{ \mathcal{D} \frac{\partial P(x, t)}{\partial x} \right\} \\ &= -\frac{1}{2} \int_{-\infty}^{\infty} dx \frac{\mathcal{D}}{P(x, t)} \left[\frac{\partial P(x, t)}{\partial x} \right]^2. \end{aligned} \quad (14.50)$$

From the definition (14.28) $\mathcal{D} > 0$. Since $P(x, t) > 0$ we conclude

$$\frac{d\mathcal{S}_B}{dt} = -\frac{d}{dt} \langle \ln P(x, t) \rangle \geq 0. \quad (14.51)$$

The magnitude \mathcal{S}_B defined in (14.47) is called *entropy*, and the result (14.51) represents the so-called *H-theorem* of Boltzmann applied to the FPK equation (Note 14.6).

The *H-theorem* is a specific signature of kinetic equations. We can consider the existence of the property (14.51) as an indication of a 'normal form' of the kinetic equations. At the equilibrium \mathcal{S}_B reaches its maximum and $\dot{\mathcal{S}}_B = 0$.

The description of dynamic systems with chaotic trajectories needs more sophisticated types of kinetics for which the divergent form does not exist and/or the inequality (14.51) may not be valid. All these topics will be discussed in the forthcoming chapters (see also Problem 14.4).

14.6 Kolmogorov conditions and conflict with dynamics

A perfect mathematical scheme often has constraints which limit its application to real phenomena. Constraints related to the Kolmogorov conditions (14.25) are very important for all problems related to the anomalous transport that will be discussed in the forthcoming chapter. Consider the limit $\delta t \rightarrow 0$ and an infinitesimal displacement δx along a particle trajectory that corresponds to this limit. Then $\delta x / \delta t \rightarrow v$ where v is the particle velocity, and the conditions (14.25) with the notation (14.28) gives

$$\frac{(\delta x)^2}{\delta t} = v^2 \delta t = \mathcal{D} = \text{const.} \quad (14.52)$$

This means that v should be infinite in the limit $\delta t \rightarrow 0$, which makes no physical sense.

Another manifestation of the conflict can be obtained directly from the solution (14.39) to the FPK equation. This solution satisfies the initial condition

$$P(x, 0) = \delta(x), \quad (14.53)$$

that is, a particle is at the origin at $t = 0$. For any finite time t solution (14.39) or (14.43) has non-zero probability of the particle to be at any arbitrary distant point x , which means the same: the existence of infinite velocities to propagate from $x = 0$ to $x \rightarrow \infty$ during an arbitrary small time interval t . A formal acceptance of this result appeals to the exponentially small input from the propagation with infinite velocities. A physical approach to the obstacle in using the FPK equation is to abandon the limit $\Delta t \rightarrow 0$ in (14.25), to introduce $\min \Delta t$, and to consider a limit

$$\frac{t}{\min \Delta t} \rightarrow \infty. \quad (14.54)$$

A more serious question is how to use (14.54) and how the FPK equation can be applied to real dynamics. Let us demonstrate the answer using the standard map (5.13) as an example.

As was mentioned in Section 5.2, the map (5.13) corresponds to a periodically kicked particle dynamics, that is, $\min \Delta t = 1$ in dimensionless variables. For $K \gg 1$ one can consider variable x to be random with almost uniform distribution in the interval $(0, 2\pi)$ (Note 14.7). Then

$$\begin{aligned} \langle \langle \sin x \rangle \rangle &= 0, & \langle \langle \sin^2 x \rangle \rangle &= \frac{1}{2} \\ \Delta p_n \equiv p_{n+1} - p_n, & \langle \langle \Delta p_n \rangle \rangle &= 0, & \langle \langle (\Delta p_n)^2 \rangle \rangle &= \frac{K^2}{2}, \end{aligned} \quad (14.55)$$

where double brackets $\langle \langle \dots \rangle \rangle$ means averaging over x , and one can write the corresponding FPK equation with respect to the slowly varying momentum p :

$$\frac{\partial P(p, t)}{\partial t} = \frac{1}{2} \mathcal{D}(K) \frac{\partial^2 P(p, t)}{\partial p^2} \quad (14.56)$$

with

$$\mathcal{D}(K) = \frac{K^2}{2}. \quad (14.57)$$

Equation (14.56) provides the normal transport. Particularly

$$\langle p^2 \rangle = \frac{1}{2} K^2 t. \quad (14.58)$$

More sophisticated analysis gives for $\mathcal{D}(K)$ an oscillating behaviour

$$\mathcal{D}(K) = K^2 \left(\frac{1}{2} - J_2(K) \right) \quad (14.59)$$

with $J_2(K)$ as the Bessel function. Due to the presence of the Bessel function, the diffusion coefficient $\mathcal{D}(K)$ oscillates as a function of K . The oscillations were observed numerically in Chirikov (1979). Their theory is known as the

Rechester-White diffusion. It keeps the same equation (14.56), and changes only $\mathcal{D}(K)$. (See Rechester and White (1980); Rechester *et al.* (1981)). More serious changes to the diffusional equation will be discussed in Chapter 16. Our main goal here is to show how the described conflict can be eliminated using truncated distributions.

14.7 Truncated distributions

A general scheme to perform a simulation of the problem of diffusion and transport for given dynamical equations is to select a set of initial points in phase space $\{x_0, p_0, t = 0\}$ and let them move until a large time t . Then for different time instants t_1, t_2, \dots, t one can collect points into bins located in phase space and create a distribution function $P(x, p, t_j)$ or its projections $P(x, t_j)$, $P(p, t_j)$. All these distributions are always truncated by some values x_{\max} , and p_{\max} because velocities of trajectories for all initial conditions are bounded during the finite time interval $(0, t)$. For a fairly large t we can split, for example, $P(p, t)$ into two parts:

$$P(p, t) = P_{\text{core}}(p, t) + P_{\text{tail}}(p, t) \quad (14.60)$$

and calculate the corresponding moments

$$\langle p^m \rangle = \langle p^m \rangle_{\text{core}} + \langle p^m \rangle_{\text{tail}}. \quad (14.61)$$

Let us estimate the second term in (14.61).

Assume that p^* is the point of splitting of $P(p, t)$ into the core and tail parts. Then

$$\langle p^m \rangle_{\text{tail}} = \int_{p^*}^{p_{\max}} dp p^m P(p, t) < (p_{\max})^m P(p^*, t). \quad (14.62)$$

For the Gaussian distribution $P(p^*, t)$ is exponentially small and we can neglect $\langle p^m \rangle_{\text{tail}}$ independently on m . This resolves the paradox with the Kolmogorov conditions for the solutions of Gaussian type. The situation is different if for large values of p the distribution function behaves algebraically, that is,

$$P(p, t) \sim \frac{c(t)}{p^{\delta_p}}, \quad (p \rightarrow \infty). \quad (14.63)$$

All moments $\langle p^m \rangle$ diverge for $m \geq \delta_p - 1$ and estimate (14.62) should be replaced by

$$\langle p^m \rangle_{\text{tail}} = \frac{c(t)}{m - \delta_p + 1} p_{\max}^{m - \delta_p + 1} \rightarrow \infty, \quad (p_{\max} \rightarrow \infty). \quad (14.64)$$

Expression (14.64) shows that for the truncated distribution with an algebraic asymptotics, the time evolution of fairly large moments is defined through the

largest value of momentum that a particle can obtain during its dynamics. The result imposes some constraints on how large can m be for the given model with its δ_p and for a selected observation time t . Opposite to the Gaussian case, we can neglect $\langle p^m \rangle_{\text{core}}$ in (14.61).

A similar statement exists for the coordinate distribution function $P(x, t)$ if its behaviour is algebraic for large $x > 0$, that is,

$$P(x, t) \sim \frac{c(t)}{x^{\delta_x}}, \quad (x \rightarrow \infty). \quad (14.65)$$

This consideration will be important when we consider anomalous transport in Chapter 16.

The distribution defined as

$$P(p, t) = \begin{cases} P^{(\text{tr})}(p, t), & 0 < p \leq p_{\text{max}}, \\ 0, & p > p_{\text{max}} \end{cases} \quad (14.66)$$

will be called *truncated distribution*, and the corresponding moments will be called *truncated moments*. Any kind of simulations of the direct dynamics deal only with the truncated distributions and moments.

Finally, we arrive at the following important constraints which are necessary for a realistic analysis of the dynamics:

$$\delta t \geq \delta t_{\text{min}}, \quad (x, p) \leq (x_{\text{max}}, p_{\text{max}}) \quad (14.67)$$

which means the infinitesimal time is bounded from below and the phase space variables are bounded from above. Other consequences of the truncation can be found in Ivanov *et al.* (2001).

Notes

Note 14.1

There exist plenty of books and papers that provide excellent presentations of the origin and improvement of the contemporary kinetic theory: from the original works of Boltzmann (1872, 1895, 1898); Ehrenfest and Ehrenfest (1911); Smolukhowski (1915); and Einstein (1905), to more sophisticated methods in Kac (1958) and Prigogine (1962). (See also the review and other references in Liboff (1998)). The transition (14.2) is known as the *random phase approximation*, and the transition (14.3) is known as the *one-particle approximation*. For more discussions, see Zaslavsky (1985).

Note 14.2

Using the properties of dynamical equations to derive a kinetic equation was first performed by Boltzmann (1872, 1895). The theory of chaotic dynamics was formally involved into kinetic theory by Zaslavsky and Sagdeev (1967)

(see also in books Zaslavsky (1985); Sagdeev *et al.* (1988); Dorfman (1999); and Lichtenberg and Lieberman (1983)).

Note 14.3

For the review of fractional kinetics and the anomalous transport in Hamiltonian dynamics, see Zaslavsky (2002b).

Note 14.4

For the review of derivation, properties, and applications of the FPK equation, see Chandrasekhar (1943) and more recently Liboff (1998).

Note 14.5

The way to derive (14.27) is slightly different from what has been used in the original works of Kolmogorov and Landau, due to the use of expansion (14.19) over δ -function and its derivatives.

Note 14.6

Boltzmann considered the expression

$$H = \langle \ln P \rangle = -S \leq 0$$

which explained the origin of the name of the H -theorem (H in Boltzmann's original work should not be confused with the Hamiltonian).

Note 14.7

In fact, in the vicinity of some arbitrary large values of K there are strong localized deviations from the uniformity. They will be considered in detail later. These deviations lead to the anomalous transport described by an equation that significantly differs from the FPK equation.

Problems

More complicated problems are marked by (*).

14.1 Derive the solution (14.39) for (14.27) with $\mathcal{D} = \text{const}$, $P(x, t = 0) = \delta(x)$, $x \in (-\infty, +\infty)$.

14.2* Find an expression for the probability $P(x_0, t_0 = 0; x_0, t)$ of the first return to a point x_0 after time t (see Risken (1989)).

14.3 Find a recurrent formula for the higher moments coefficients \mathcal{D}_m in (14.41).

14.4* Consider $\dot{\mathcal{S}}_B$ with the definition of \mathcal{S}_B in (14.47), and the distribution function $P(x, t)$ which satisfies (14.26). Find a condition of the validity of a monotonic entropy growth.