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Part I

Fundamentals of nonequilibrium statistical mechanics

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Basic issues in nonequilibrium statistical mechanics

Perhaps due to its technical complexity, oftentimes one sees in research papers on nonequilibrium quantum field theory (NEqQFT) more emphasis placed on the field-theoretical formalisms than the ideas these sophisticated techniques attempt to capture, or the issues such problems embody. All the more so, we need some basic understanding of the important issues and concepts in nonequilibrium statistical mechanics (NEqSM), and how they are manifested in the context of quantum field theory. Many important advances in this field came from asking such questions and finding out how to answer them in the language of quantum field theory. Because of this somewhat skewed existing emphasis in NEqQFT, and since we do not assume the reader to have had a formal course on NEqSM before, we shall give a brief summary of the basic concepts of NEqSM relevant to the field-theoretical processes discussed in this book. Many fine monographs and reviews written on this subject take a more formal mathematical approach. Since our purpose here is to familiarize readers with these issues and their subtleties, rather than training them to work in the rich field of NEqSM (which includes in addition to the traditional subject matter such as the projection operator formalism and open system concepts, also current topics at their foundation, such as dynamical systems and quantum chaos), we choose to approach these topics in a more intuitive and physical way, sacrificing by necessity rigor and completeness.

We first examine some commonly encountered physical processes and try to bring out in each a different key concept in NEqSM. To have a concrete bearing and a common ground, let us focus on just one such issue which is of paramount importance and poses a constant challenge to theoretical physicists: How does apparent irreversibility in the macroscopic world arise from the time-reversal invariant laws of microphysics [Leb93, HaPeZu94, Mac92, Sch97]?

We begin with an analysis of the nature and origin of irreversibility in well-known physical processes such as dispersion (referring in the specific context here to the divergence of neighboring trajectories in configuration or phase space due to dynamical instability), diffusion, dissipation and mixing. We will seek the microdynamical basis of these processes and clarify the distinction between processes whose irreversibility arises from the stipulation of special initial conditions, and those arising from the system's interaction with a coarse-grained environment. It is beneficial to keep in mind these processes and the issues they embody when we begin our study of quantum field processes so that they will not be marred by the technical complexity of quantum field theory. We

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can ask questions such as (1) "What is the entropy generation from particle creation in an external field or a dynamical spacetime, as in cosmology?"; (2) "How could an interacting field thermalize?"; (3) "Is there irreversibility associated with quantum fluctuations in field theoretical processes like particle creation?" Or, more boldly, "Can the 'birth of the Universe' be viewed as a large fluctuation?" "Might it not happen at all – a 'still' birth – due to the powerful dissipative effects of particle creation which suppresses the tunneling rate?" (4) "Can one use thermodynamic relations to characterize certain quantum field processes?"

These questions reveal how deeply one can probe into the NEqSM features of quantum field theory and how quantum field processes can lend themselves to statistical mechanical and thermodynamic depiction or characterization. Asking question (1) reveals the differences resulting from many levels of coarse graining between a quantum field understanding of particle creation processes (no entropy production because the vacuum is a pure state) and a thermodynamic description (yes, entropy is proportional to the number of particles produced). Asking question (2) forces us to reckon with the intricate NEqSM features of an interacting quantum field such as how a correlation entropy can be defined from the Schwinger–Dyson hierarchy. These aspects are not usually discussed in quantum field theory textbooks. The first part of question (3) brings out the often used yet poorly understood aspects of noise – beginning with quantum noise associated with vacuum fluctuations, properties of multiplicative colored noise, and nonlocal dissipation and their effects on the dynamical processes. The second part of question (3) is the so-called "back-reaction" effect of quantum fields on a background field or background spacetime. Question (4) asks if this effect can have a thermodynamic interpretation. To the degree that thermodynamics is the long-wavelength, heavily coarse-grained limit of microphysics and quantum field theory is a theory of microphysics, we certainly expect such relations to exist and their discovery will reveal the relation between micro–macro and quantum-to-classical transitions. A well-known relation is the black hole thermodynamics of Bekenstein [Bek73] and the quantum Hawking radiation [Haw75]. Sciama [Sci79] suggested that this can be understood from the viewpoint of quantum dissipative systems. This view also applies to dissipation of anisotropy in the early universe due to particle creation from the vacuum. We will find out later that both for the black hole and the early universe these processes can indeed be understood as manifestations of a fluctuation–dissipation relation, relating fluctuations of quantum fields to dissipation in the dynamics of the background field or spacetime.

1.1 Macroscopic description of physical processes

Let us begin by examining a few examples of irreversible processes to illustrate their different natures and origins. Consider the following processes:

Dispersion
Diffusion
Dissipation
Relaxation
Mixing
Recurrence
Decoherence
Recoherence

They contain different aspects of irreversibility. The usage of these terms appearing in general-purpose books could be rather loose or even confusing. For example, diffusion, relaxation and dissipation are often seen used interchangeably. Even the same word could mean different things in different contexts. For example, classical diffusion is often viewed as a form of dissipation, while quantum diffusion refers to phase dispersion, usually occurs at a much faster time-scale and is more closely related to decoherence than dissipation. We will discuss quantum phenomena in Chapter 3. Here we will focus on the first six such processes listed above and aim at providing some microdynamics basis to these processes in order to give them a more precise meaning. In so doing we hope to elucidate some basic notions and issues of NEqSM through examples.

We first highlight the distinction between dissipative processes (which are always irreversible) and irreversible or "apparently" irreversible processes (which are not necessarily dissipative). For example, in elastic scattering, neighboring trajectories diverge exponentially fast. This is characteristic of mixing systems, which are reversible. Relaxation and diffusion referring to dissipative systems are irreversible. They are mixing systems with some type of coarse graining introduced. As we shall see, not any type of coarse graining leads to irreversibility. Many factors enter, such as the large size of the system, the particular initial conditions chosen, or the time-scales at work. This is where it calls for special caution in doing the analysis. Better understanding of the chaotic behavior in classical molecular dynamics has provided a firmer microscopic basis for nonequilibrium statistical mechanics. Such studies for quantum systems are less developed and for this reason we shall refrain from describing them. In Chapter 3 we shall have occasion to discuss quantum decoherence and dissipation where the interplay of quantum and thermal fluctuations in the environment and their effects on the system will be discussed. We shall also revisit these issues of irreversibility and approach to equilibrium in Chapter 12.

A. Dispersion

Consider a system of dilute gas made up of interacting particles modeled as hard spheres with diameter d. For simplicity, let us work in two dimensions with hard disks. (Our illustration here follows [Gas98]; see also [Ma85] which contains excellent conceptual discussions.) Assume the particles move with constant velocity v

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and traverse a distance given by the mean free path $\ell \gg d$ before colliding with another particle elastically. The trajectory of any particle governed by the laws of mechanics is of course reversible in time. However, upon just a few collisions two neighboring trajectories will deviate from each other very rapidly if the scattering surface is convex, as a sphere is. To see this, let's set our stop watch time zero ($t = 0$) right after the first collision (call this collision the $n = 0$ one) and follow the particle's trajectory for n subsequent collisions. Call the scattering angle of the first collision $\theta(0)$ and the uncertainty associated with it $\delta\theta(0)$ and likewise for the scattering angle after an additional n collisions $\theta(t)$ and its uncertainty $\delta\theta(t)$. For each additional collision the uncertainty in the scattering angle increases by a factor of ℓ/d deduced from the simple trigonometry of incident and scattered trajectories. So after n collisions then

$$|\delta\theta(t)| \sim |\delta\theta(0)|^n \equiv |\delta\theta(0)| e^{\lambda t} \tag{1.1}$$

The second equivalence relation above defines the parameter λ, which is called the Lyapunov exponent (actually its maximal value enters into this expression). The time for n successive collisions is given by $t = n\tau$ where τ is the time between collisions related to the mean free path ℓ by $v = \ell/\tau$. Thus the (maximal) Lyapunov exponent is given by

$$\lambda \sim \frac{1}{\tau} \ln \frac{\ell}{d} \tag{1.2}$$

This simple way of estimating the maximum Lyapunov exponent first given by Krylov [Kry44, Kry79] remains very useful in illustrating the elemental process of divergence of neighboring trajectories due to dynamical instability, referred to here as "dispersion" for short. For hard sphere collisions we see that after a sufficiently long time $|\delta\theta(t)| \approx 1$, the exit direction becomes completely indeterminate due to the accumulated error.

The asymmetry in the initial and final conditions of the collection of trajectories (congruence) comes from the accumulation and magnification of the *uncertainty in the initial conditions* due to the collisions, even though the dynamical law governing each trajectory is time-symmetric. To trace a particular trajectory backwards in time after a large number of collisions requires an exponentially high degree of precision in the specification of the initial condition. This ultra-sensitivity of dynamics to initial conditions is characteristic of chaotic systems. Note that the divergence of neighboring trajectories in phase space or parameter space is an intrinsic property of the nonlinear Hamiltonian of the system, not a result of coarse graining by the truncation of the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) series *and* the causal factorizability of the two-particle correlation function as in Boltzmann's molecular chaos hypothesis. (Initially uncorrelated particles become correlated after collisions, thus giving rise to time-asymmetry in the dissipative dynamics of Boltzmann's equation.) The evolution of an ensemble

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of such systems at some finite time from the initial moment often appears to be unrelated to their initial conditions, not because the individual systems are insensitive to the initial conditions but because they are overly-sensitive to them, thus making it difficult to provide an accurate prediction of each system's state in the future. It is in this sense that these systems manifest irreversibility. In contrast, for an integrable system the trajectories stay close to each other because the regions in phase space for its dynamics are limited by the constants of motion. Such trajectories in integrable systems are referred to as "stable" while those in chaotic systems are "unstable" as they become dispersive in the sense defined above owing to their dynamical instability. We will return in a later section to irreversibility and nonequilibrium thermodynamics considered from the framework of Hamiltonian dynamics.

B. Diffusion

Let us look at some simple examples in kinetic theory: gas expansion, ice melting and an ink drop in water. These are irreversible processes because the initial states of 10^{23} molecules on one side of the chamber and a piece of ice or ink drop immersed in a bath of water are *highly improbable configurations* out of all possible arrangements. These initial conditions are states of very low entropy. The only reason why they are special is because we arrange them to be so. For these problems, we also know that the system–environment separation and interaction make a difference in the outcome. In the case of an expanding ideal gas, for example, for free expansion the change of entropy is $\delta S_{\text{system}} > 0, \quad \delta S_{\text{environ}} = 0, \quad \delta S_{\text{total}} > 0$. For isothermal *quasistatic* expansion: $\delta S_{\text{system}} = -\delta S_{\text{environ}} > 0, \quad \delta S_{\text{total}} = 0$ instead (see, e.g. [Rei65]).

Another important factor in determining whether a process is irreversible is the *time-scale* of observation compared to the dynamic time-scale of the process. We are familiar with the irreversible process of an ink drop dispersing in water which happens in a matter of seconds, but the same dye suspension put in glycerine takes days to diffuse, and for a short duration after the initial mixing (say, by cranking the column of glycerine with a vertical stripe of dye one way) one can easily "unmix" them (by reversing the direction of cranking [UMDdemo]). We will discuss in the next section under what conditions and in what sense a "mixing" system, though time-reversible, can be viewed as capable of approaching equilibrium. Diffusion, when used in the sense of dissipation, is nevertheless an irreversible process.

C. Dissipation

There are two basic models of dissipation in nonequilibrium statistical mechanics: the Boltzmann kinetic theory of dilute gas, and the Langevin theory of Brownian motion. Each invokes a different set of concepts, and even their relation is illustrative. In kinetic theory, the equations governing the n-particle distribution functions (the BBGKY hierarchy) preserve the full information of an

n-particle system. It is (1) ignoring (more often restricted by the precision of one's observation than by choice) the information contained in the higher-order correlations (truncation of the BBGKY hierarchy), *and* (2) the imposition of causal factorization conditions, like the molecular chaos assumption, that brings about dissipation and irreversibility in the dynamics of the lower-order correlations [Zwa01, Bal75].

In the lowest order truncation of the BBGKY hierarchy valid for the description of dilute gases, the Liouvillian operator L acting on the one-particle distribution function $f_1(r_1, p_1, t)$ is driven by a collision integral involving a two-particle distribution function $f_2(r_1, p_1, r_2, p_2, t)$ (cf. Chapters 2 and 11). Boltzmann's molecular chaos ansatz (MCA) assumes an initial uncorrelated state between two particles: $f_2(1,2) = f_1(1)f_1(2)$, i.e. that the probability of finding particle 1 at (r_1, p_1, t) and particle 2 at (r_2, p_2, t) at the same time t is equal to the product of the single-particle probabilities (a factorizable condition). Note that this condition is assumed to hold only initially, but not finally. A short-range interaction in a collision process will almost certainly generate dynamical correlations between the two collision partners. The truncated BBGKY hierarchy (with MCA) is an example of what we call an effectively open system (see Section 1.5 of this chapter). Boltzmann's explanation of dissipation in macroscopic dynamics is one of the crowning achievements of theoretical physics.

Dissipation in an open system described by the Langevin dynamics has similarities with and differences from that of an effectively open system (as exemplified by the Boltzmann system). The open system can be one distinguished oscillator, the Brownian particle (with mass M), interacting with many oscillators (with mass m) serving as its environment (see Chapter 2). Dissipation in the dynamics of the open system arises from ignoring details of the environmental variables and only keeping their averaged effect on the system (this also brings about a renormalization of the mass and the natural frequency of the Brownian particle). Usually one assumes $M \gg m$ and weak coupling between the system and the environment to simplify calculations. The effect of the environment on a particular system can be summarized by its spectral density function, but other environments can produce equivalent effects. In both of these models, as well as in more general cases, the following conditions are essential for the appearance of dissipation (see, e.g. [Hu89]):

(a) *System–environment separation.* This split depends on what one is interested in, which defines the system: it could be the slow variables, the low modes, the low order correlations, the mean fields; or what one is restricted to: the local domain, the late history, the low energy, the asymptotic region, outside the event horizon, inside the particle horizon, etc.

(b) *Coupling.* The environment must have many degrees of freedom to share with and spread the information from the system; its coupling with the system

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must be effective in the transfer of information (e.g. nonadiabatic) and the response of the coarse-grained environment must be sufficiently nonsystematic in that it will only react to the system in an incoherent and retarded way. (An example of almost the opposite condition is a dressed atom, i.e. an atom in a high finesse electromagnetic cavity where the quantum coherence of the system can be preserved to a high degree [CoPaPe95].)

(c) *Coarse graining.* One must ignore or down-grade the full information in the environmental variables to see dissipation appearing in the dynamics of the open system. (The time of observation enters also, in that it has to be greater than the interaction time of the constituents but shorter than the recurrence time in the environment.) Coarse graining can be the causal truncation of a correlation hierarchy, the averaging of the higher modes, the "integrating out" of the fluctuation fields, or the tracing of a density matrix (discarding phase information).

(d) *Initial conditions.* Whereas a dissipative system is generally less sensitive to the initial conditions in that for a wide range of initial states dissipation can drive the system to the same final (equilibrium) state, the process is nevertheless possible only if the initial state is off-equilibrium. The process manifests irreversibility also because the initial time is singled out as a special temporal reference point when the system is prepared in that particular initial state. Thus in this weaker sense, dissipation is also a consequence of specially prescribed initial conditions.[1]

While the dynamics of the combined system made up of a subsystem and its environment is unitarity, and its entropy remains constant in time, when certain coarse graining is introduced in the environment, the subsystem turns into an open system, and the entropy of this open system (constructed from the reduced density matrix by tracing out the environmental variables) increases in time. In this open system dynamics, the effect of the coarse-grained environment on the subsystem leads to dissipation and irreversibility in its dynamics.

In our prior discussion of dynamical instability or "dispersion" with the example of hard-disk scattering we were introduced to irreversible but nondissipative processes. Irreversibility there refers to the ultra-sensitivity of the dynamics to the initial conditions. It is extremely difficult to trace back in time a highly divergent congruence of trajectories. The source of irreversibility

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[1] Note the distinction between these cases: If one defines t_0 as the time when a dissipative dynamics begins and t_1 as when it ends, then the dynamics from t_0 to $-t$ is exactly the same as from t_0 to t, i.e. the system variable at $-t_1$ is the same as at t_1. This is expected because of the special role assigned to t_0 in the dynamics with respect to which there is time-reversal invariance, but it is not what is usually meant by irreversibility in a dissipative dynamics. The arrow of time there is defined as the direction of increase of entropy and irreversibility refers to the inequivalence of the results obtained by reversing t_0 and t_1 (or, for that matter reversing t_0 and $-t_1$), but not between t_1 and $-t_1$. The time-reversal invariance of the H-theorem has the same meaning.

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there is by nature fundamentally different from that found in open systems discussed here. The former dynamics is irreversible but nondissipative, while the latter is both dissipative and irreversible. Both types of processes depend on the stipulation of initial conditions. The difference is that the former depends sensitively so, the latter less sensitively. Thus dissipative processes must involve some measure of coarse graining, but coarse graining alone need not lead to dissipation. We will have a subsection later on the issue of coarse graining.

D. Phase mixing

Two well-known effects fall under this category: Landau damping and spin echo (e.g. [Bal75, Ma85]). Let us examine the first example. If one considers long-ranged forces such as the Coulomb force in a dilute plasma gas where close encounters and collisions are rare, the factorizable condition can be assumed to hold throughout, before and after each collision (thus there is no causal condition like the molecular chaos assumption imposed). Under these conditions the Boltzmann kinetic equation becomes a Vlasov (or collisionless Boltzmann) equation (see, e.g. [Bal75, Kre81]). This problem will be discussed in Chapters 10 and 11. The dependence on the one-particle distribution function $f_1(\mathbf{r}, \mathbf{p}, \mathbf{t})$ makes the Vlasov equation nonlinear, and it has to be solved in a self-consistent way. (This aspect is analogous to the Hartree approximation in many-body theory.) Note that the Vlasov equation which has a form depicting free streaming is time-reversal invariant: the Vlasov term representing the effect of the averaged field does not cause dissipation. This mean-field approximation in kinetic theory, which yields a unitary evolution of reversible dynamics, is, however, only valid for times short compared to the relaxation time of the system in its approach to equilibrium. This relaxation time is associated with the collision-induced dissipation process.

Landau damping in the collective local charge oscillations, being a solution of the Vlasov equation, is intrinsically a reversible process. The appearance of apparent “irreversibility” is a consequence of some specially stipulated initial conditions. One may even be able to find a function which is monotonically increasing and refer to it as representing entropy generation. However, upon the choice of some other condition, this feature can disappear and the entropy function can decrease. (An example in Chapter 4 is the entropy function defined in the particle number basis.) Landau “damping” is a mixing process, illustrated here by the Vlasov dynamics. It is fundamentally different from the dissipation process, in that the latter has an intrinsic damping time-scale but not the former, and that while dissipation depends only weakly on the initial conditions, mixing is very sensitive to the initial conditions. Spin echo is another well-known example of phase mixing [Bal75]. For quantum plasma, one needs to coarse grain the phase information in the wavefunctions *and* consider special initial conditions to see this apparent “damping” effect (more in Chapter 4).

From the array of examples above we see that irreversibility and dissipation involve very different causes. The effect of interaction, the role of coarse graining, the choice of time-scales, and the specification of initial conditions in any process can give rise to very different results. We will expand on these physical conditions later, after we have had a chance to look at the microscopic characterization of these macroscopic processes, i.e. their molecular dynamics basis.

1.2 Microscopic characterization from dynamical systems behavior

From a sampling of these macroscopic processes we see a variety of physical behavior. The underlying causes should all be traceable to the microscopic molecular dynamics, to which we now turn our attention. Let us start with a deceptively simple question: An isolated mechanical system is time-reversible. Under what conditions and in what sense does a large isolated system reach equilibrium?

1.2.1 Ergodicity describes a system in equilibrium

An isolated system of N molecules in a volume V has a constant total energy E under the Hamiltonian $H(\mathbf{r}, \mathbf{p})$, where $\mathbf{r}, \mathbf{p}$ each is a $3N$-dimensional vector denoting the position and momenta of all the particles in a $6N$-dimensional phase space Γ. The density function $\rho(\gamma)$ is defined such that the probability of finding a member γ of the ensemble in a differential volume $d\Gamma \equiv d\mathbf{r}_1 \cdots d\mathbf{r}_N d\mathbf{p_1} \cdots \mathbf{dp_N}$ is equal to $\rho(\gamma) d\Gamma$. Its dynamics is described by the **flow** of each member of the ensemble restricted to the constant energy surface or manifold $\mathcal{E}$ in Γ. Since the number of members flowing in and out of a region in phase space should be equal for all times we have ρ satisfying the Liouville equation,

$$\frac{d\rho}{dt} \equiv \frac{\partial \rho}{\partial t} + \sum_1^N \left(\dot{\mathbf{r}}_i \cdot \frac{\partial}{\partial \mathbf{r}_i} + \dot{\mathbf{p}}_i \cdot \frac{\partial}{\partial \mathbf{p}_i} \right) \rho = 0 \tag{1.3}$$

where an overdot denotes derivative with respect to time.

In statistical mechanics the microcanonical **ensemble** describes such an isolated system. The number of states is represented by the area of the energy surface E in phase space:

$$\Omega(E) = \int_{H=E} d\mu \equiv \int_\Gamma \delta(H - E) d\mu, \tag{1.4}$$

where μ is the invariant measure on Γ. The entropy is defined as $S = k_\mathrm{B} \ln \Omega(E)$. The ensemble average of a phase space function F over the energy surface E is given by

$$\langle F \rangle_\mu \equiv \frac{\int_{H=E} d\mu F(\gamma)}{\int_{H=E} d\mu} = \frac{\int_\Gamma F(\gamma) \delta(H - E) d\mu}{\int_\Gamma \delta(H - E) d\mu} \tag{1.5}$$