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Thermodynamics and dynamics of systems with long-range interactions

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ABSTRACT

We review simple aspects of the thermodynamic and dynamical properties of systems with long-range pairwise interactions (LRI), which decay as $1/r^{d+\sigma}$ at large distances r in d dimensions. Two broad classes of such systems are discussed. (i) Systems with a slow decay of the interactions, termed "strong" LRI, where the energy is super-extensive. These systems are characterized by unusual properties such as inequivalence of ensembles, negative specific heat, slow decay of correlations, anomalous diffusion and ergodicity breaking. (ii) Systems with faster decay of the interaction potential, where the energy is additive, thus resulting in less dramatic effects. These interactions affect the thermodynamic behavior of systems near phase transitions, where long-range correlations are naturally present. Long-range correlations are often present in systems driven out of equilibrium when the dynamics involves conserved quantities. Steady state properties of driven systems with local dynamics are considered within the framework outlined above.

1. Introduction

This paper provides a brief introduction to the thermodynamics and dynamics of systems with long-range interactions (LRI). In these systems, the interaction potential between the constituent particles decays slowly with distance, typically as a power law $\sim 1/r^{d+\sigma}$ at large separation $r \gg 1$, where d is the spatial dimension. The interaction potential may be isotropic or anisotropic (as in magnetic or electric dipolar systems). Long-range interacting systems may be broadly classified into two groups: those with $-d \leq \sigma \leq 0$, which are termed systems with "strong" LRI, and those with positive but not too large σ, which are termed systems with "weak" LRI. Systems with strong LRI show significant and pronounced dynamic and thermodynamic effects due to the slow decay of the interaction potential. In contrast, in systems with weak LRI, the potential decays relatively faster, resulting in less pronounced effects. For a recent review on long-range interacting systems, see Ref. [1].

Long-range interacting systems are rather common in nature, for example, self-gravitating systems ($\sigma = -2$) [2], non-neutral plasmas ($\sigma = -2$) [3], dipolar ferroelectrics and ferromagnets (anisotropic interactions with $\sigma = 0$) [4], two-dimensional geophysical vortices ($\sigma = -2$) [5], wave-particle interacting systems such as a free-electron laser [6], and many others.

Let us first consider systems with strong LRI. These systems are generically non-additive, resulting in many unusual properties, both thermal and dynamical, which are not exhibited by systems with weak LRI or with short-range interactions. For example, the entropy may turn out to be a non-concave function of energy, yielding negative specific heat within the microcanonical ensemble [7–14]. Since canonical specific heat is always positive, it follows that the two ensembles need not

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be equivalent. More generally, the inequivalence is manifested whenever a model exhibits a first-order transition within the canonical ensemble [15,16]. Non-additivity may also result in breaking of ergodicity, where the phase space is divided into domains. Local dynamics do not connect configurations in different domains, leading to finite gaps in macroscopic quantities such as the total magnetization in magnetic systems [17–23].

Studies of relaxation processes in models with strong LRI have shown that a thermodynamically unstable state relaxes to the stable equilibrium state unusually slowly over a timescale which diverges with the system size [5,17,24–30]. This may be contrasted with the relaxation process in systems with short-range interactions. Diverging timescales in systems with strong LRI result in long-lived quasistationary states. In the thermodynamic limit, these states do not relax to the equilibrium state, so that the system remains trapped in these states forever. These quasistationary states and their slow relaxation have been explained theoretically in the framework of kinetic theory [3,5,28–31]. Recent progress in the kinetic theory of systems with long-range interactions [31–33] has also uncovered algebraic relaxation and explained anomalous diffusion in and out of equilibrium.

It is worthwhile to point out that non-additivity may occur even in finite systems with short-range interactions in which surface and bulk energies are comparable. Negative specific heat in small systems (e.g., clusters of atoms) has been discussed in a number of studies [34–37].

Systems with weak LRI, for which $\sigma > 0$, are additive. Unless one is in the vicinity of a phase transition, their thermodynamic properties are similar to those with short-range interactions, e.g., the specific heat is non-negative, and the various statistical mechanical ensembles are equivalent. Near a phase transition, long-range correlations build up. These correlations affect the universality class of a system near a continuous phase transition, resulting in critical exponents which depend on the interaction parameter σ. Moreover, for these systems, the upper critical dimension $d_c(\sigma)$ above which the critical behavior becomes mean-field-like depends on σ and has a smaller value than in systems with short-range interactions for which $d_c = 4$, see Refs. [38,39]. A system with weak LRI may exhibit phase transitions in one dimension at a finite temperature, which are otherwise forbidden in a system with short-range interactions [40,41].

So far we have discussed systems in equilibrium. Long-range correlations may also build up in driven systems which reach a non-equilibrium steady state that violates detailed balance. Quite generally, such steady states in systems with conserving dynamics exhibit long-range correlations, even with local dynamics. One thus expects peculiarities in behavior of equilibrium systems with long-range interactions to also show up in steady states of non-equilibrium systems with conserving local interactions. An example of such a non-equilibrium system with long-range correlations is the so-called *ABC* model. In this model, three species of particles, *A*, *B* and *C*, move on a ring with local dynamical rules. At long times, the system reaches a nonequilibrium steady state in which the three species are spatially separated. The dynamics of this model lead to effective long-range interactions in the steady state [42,43].

The paper is laid out as follows. In Section 2, we discuss the thermodynamics and dynamics of systems with strong long-range interactions. This is followed by a discussion on upper critical dimension for systems with weak LRI in Section 3. The *ABC* model, exhibiting long-range correlations under out-of-equilibrium conditions is discussed in Section 4. The paper ends with conclusions.

2. Strong long-range interactions

2.1. Thermodynamics

Here we briefly discuss some general thermodynamic properties of systems with strong LRI. These systems are non-extensive and non-additive. For example, the energy of a particle interacting with a homogeneous distribution of particles in a volume V scales as $V^{-\sigma/d}$, so that the total energy scales superlinearly with the volume as $V^{1-\sigma/d}$, making it non-extensive, and hence, non-additive.

The most immediate consequence of non-additivity is that, unlike short-range systems, the entropy S is not necessarily a concave function of energy. This may be understood by referring to Fig. 1. The equilibrium state at a given energy within a microcanonical ensemble is obtained by maximizing the entropy at that energy. A short-range interacting system is unstable in the energy interval $E_1 < E < E_2$, since it can gain in entropy by phase separating into two subsystems with energies E_1 and E_2, keeping the total energy fixed. The energy and entropy densities are then given by the weighted average of the corresponding densities of the two coexisting subsystems. As a result, the physically realizable entropy curve in the unstable region is obtained by the common tangent line, resulting in an overall concave curve. However, in systems with strong LRI, due to non-additivity, the energy density of two coexisting subsystems is not given by the weighted average of the energy density of the two subsystems. Therefore, the non-concave curve of Fig. 1 could, in principle, represent a physically realizable stable system, with no occurrence of phase separation. This results in a microcanonical negative specific heat in the interval $E_1 < E < E_2$ [7–11,14]. Since the specific heat within the canonical ensemble is always positive, being given by the fluctuations about the mean of the system energy, this leads to inequivalence of ensembles, which is particularly manifested whenever a first-order transition with coexistence of two phases is found within the canonical ensemble [15,16].

Another feature related to non-additivity is that of a discontinuity in temperature at a first-order phase transition within a microcanonical ensemble, say, from a paramagnetic to a magnetically ordered phase. This may be understood by referring to Fig. 2(a), which shows the entropy $S(M, E)$ as a function of the magnetization M at an energy E close to the transition. It exhibits three local maxima, one at $M = 0$ and two other degenerate maxima at $M = \pm M_0$. As the

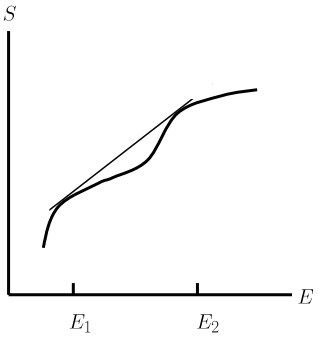

Fig. 1. Entropy as a non-concave function of energy. For short-range systems, due to additivity, the physically realizable curve in the interval $E_1 < E < E_2$ is given by the common tangent line, resulting in an overall concave curve. In systems with long-range interactions, the non-concave curve may be actually realizable, giving rise to negative microcanonical specific heat.

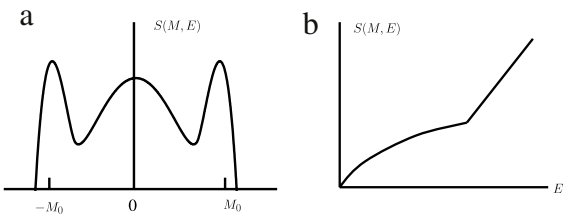

Fig. 2. (a) Entropy vs. magnetization close to a first-order transition in a magnetic system with long-range interactions. (b) Entropy vs. energy, showing a slope and hence, a temperature discontinuity at a first-order transition point.

energy varies, the heights of the peaks change. The paramagnetic phase occurs at energies such that $S(0, E) > S(\pm M_0, E)$, while the magnetically ordered phase occurs at energies where the inequality is reversed. The temperatures in the two phases are given by $1/T = \partial S(0, E)/\partial E$ and $1/T = \partial S(\pm M_0, E)/\partial E$, respectively. At the transition point, when one has $S(0, E) = S(\pm M_0, E)$, these two derivatives are generically not equal, resulting in a temperature discontinuity. This shows up in the entropy vs. energy curve, see Fig. 2(b).

The non-additive property also manifests itself in dynamical features through breaking of ergodicity, the reason for which may be traced back to the fact that in systems with strong LRI, the domain in the phase space of extensive thermodynamic variables may be non-convex. As a result, gaps may exist in phase space between two points corresponding to the same energy, so that local energy-conserving dynamics cannot take the system from one point to the other, leading to breaking of ergodicity.

The entropy S of a system, given by the number of ways of distributing N particles with total energy E in a given volume V, typically scales linearly with the volume for both short- and long-range interacting systems. The energy, on the other hand, scales superlinearly with the volume in systems with LRI. As a result, in these systems in the thermodynamic limit, the dominant contribution to the free energy $F = E - TS$ at any finite temperature T is due to the energy, resulting in a trivial thermodynamics with the ground state always representing the equilibrium state. However, there are examples of finite-sized real systems with long-range interactions (e.g., self-gravitating systems such as globular clusters, [5]) where the temperature could be sufficiently high to make the entropic term TS compete with the energy E, resulting in a non-trivial thermodynamics. To study this limit in theory, it is convenient to rescale the energy by the factor $V^{\sigma/d}$ (alternatively, rescale the temperature by $V^{-\sigma/d}$) so that the two terms in F become comparable. This was first suggested by Kac [44]. Although such rescaling makes the system extensive, it remains non-additive, leading to unusual thermodynamic properties, as mentioned above.

To illustrate some of these unusual thermodynamic behavior in systems with strong LRI, it is instructive to analyze phase diagrams of representative models. A class of models amenable to exact analysis comprises those where the long-range part of the interaction is of mean-field type. These models have been applied to study dipolar ferromagnets [45]. An example in this class is the Ising model with both long- and short-range interactions. The model considers Ising-spins $S_i = \pm 1$ on a one-dimensional lattice of N sites with periodic boundary conditions. The Hamiltonian is given by

$$H = -\frac{K}{2}\sum_{i=1}^{N}(S_iS_{i+1} - 1) - \frac{J}{2N}\left(\sum_{i=1}^{N}S_i\right)^2. \tag{1}$$

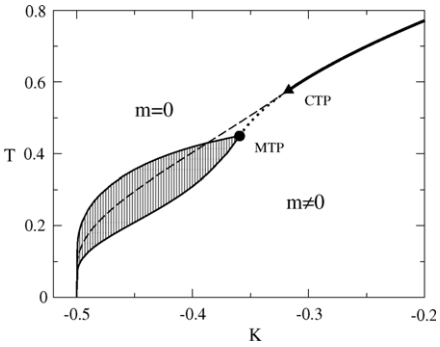

Fig. 3. The (K, T) phase diagram for the Hamiltonian in Eq. (1) within the canonical and the microcanonical ensembles. Here $J = 1$. In the canonical ensemble, the large K transition is continuous (bold solid line) down to the canonical tricritical point CTP where it turns first order (dashed line). In the microcanonical ensemble, the continuous transition coincides with the canonical one at large K (bold line). It persists at lower K (dotted line) down to the microcanonical tricritical point MTP where it becomes first order, with a branching of the transition line (solid lines). The shaded region between these two lines is not accessible.
Source: The figure is taken from Ref. [17].

Here the first term represents a nearest-neighbor coupling which could be either ferromagnetic ($K > 0$) or antiferromagnetic ($K < 0$). On the other hand, the second term, corresponding to a long-range, mean-field type interaction, is ferromagnetic, $J > 0$.

The canonical phase diagram of this model was analyzed in Ref. [46–48], while the microcanonical phase diagram was obtained in Ref. [17]. Fig. 3 shows the phase diagram in the two ensembles in the (K, T) plane with $J = 1$ and antiferromagnetic K. Here T is the temperature. We see that the microcanonical and the canonical critical lines coincide up to the canonical tricritical point CTP. The microcanonical line extends beyond this point into the region where, within the canonical ensemble, the model is magnetically ordered. In this region, the microcanonical specific heat is negative. At $K = K_{MTP}$, the microcanonical transition turns first order, with a branching of the transition line and a temperature discontinuity. The shaded region in the phase diagram represents an inaccessible domain resulting from the discontinuity in temperature.

On quite general grounds, one expects the above features of the phase diagram to be valid for any system in which a continuous transition line becomes first order at a tricritical point, for example, in the phase diagrams of the spin-1 Blume–Emery–Griffiths model [15,16], in an XY model with two- and four-spin mean-field-like ferromagnetic interaction terms [49], and in an XY model with long- and short-range, mean-field type interactions [50]. A classification of possible types of inequivalent canonical and microcanonical phase diagrams in systems with long-range interactions is given in Ref. [12].

2.2. Dynamics of Hamiltonian systems: kinetic theories

We now turn to the dynamics of systems with strong long-range interactions. The dynamics of discrete spin systems with long-range interactions will be considered in Section 2.3. Here we consider continuous Hamiltonian systems with long-range interactions. For simplicity, we limit our discussion to the following dynamical equations of motion for a system of N particles, given by

$$\begin{aligned} \dot{x}_i &= p_i, \\ \dot{p}_i &= -\frac{1}{N}\sum_{j\neq i} \frac{\mathrm{d}W(x_i - x_j)}{\mathrm{d}x_i}. \end{aligned} \tag{2}$$

Here x_i and p_i are, respectively, the coordinate and the momentum of the i-th particle and $W(x)$ is the interparticle potential. For simplicity, we first discuss the case where the potential W is of infinite range, i.e., every particle interacts with every other (mean-field interaction). The case $W(x) \sim 1/x^{d+\sigma}$, where d is the spatial dimension, is very similar, as long as $\sigma < 1$. Here the variable x is a spatial variable, similar to the variable r is the previous section. In some cases, for instance, in the HMF model discussed later (see Eq. (8)), it could also be interpreted as an internal degree of freedom. Note that, in accordance with the prescription of Kac (Section 2.1), the potential in the Hamiltonian dynamics, Eq. (2), is scaled by the factor $1/N$. This scaling factor arises from a change of timescale, and is the natural choice here, as it implies that each particle experiences a force of $O(1)$ in the limit $N \to \infty$.

In the limit of large N, the dynamical evolution given by Eq. (2) is well approximated by kinetic theories. On a relatively short timescale (that diverges with N), the evolution is described by the Vlasov equation. On a much longer timescale, the relaxation towards equilibrium is governed by the Lenard–Balescu-type dynamics (or, its approximation by the Landau equation). These equations have been applied to self-gravitating stars, plasmas in the weak-coupling limit, and point vortex models in two-dimensional turbulence [3,5,29,33,51,52].

Table 1
The Boltzmann equation on the one hand, and the Vlasov and the Lenard–Balescu equations on the other hand are obtained in two opposite limits: for the former, in the Grad limit for dilute gases (rare collisions), while, for the latter, in the limit where each particle interacts with a macroscopic number of others. The structure of the kinetic theory in both cases, however, share many analogies, as shown in the table.

Small parameter	Short-ranged dilute gases $a/l = 1/\left(\pi a^2 n\right)$	Long-range systems $1/N$
Equations:		
Initial evolution	Collisionless Boltzmann equation	Vlasov equation
Late relaxation towards equilibrium	Boltzmann equation	Lenard–Balescu equation
Vanishing correlations	Yes	Yes
Boltzmann entropy	Yes	Yes
Stosszahl Ansatz	Yes	Yes
Steady states of the initial evolution	Local Poisson distribution or local thermal equilibrium	Quasistationary states
Relaxation timescale	$\propto l/\bar{v}$ or larger	$\propto N$ or larger
Long-range temporal correlations and algebraic decays	Yes Yes	Yes Yes
Anomalous diffusion	Dimension dependent	Yes

The aim of the following subsections is to briefly present these classical kinetic equations and some recent results related to them, including predictions of quasistationary states, anomalous diffusion and algebraic relaxation. Our presentation makes a systematic parallel to the well-known case of the Boltzmann equation for short-range systems and also stresses numerous analogies between the two cases.

2.2.1. Comparison of kinetic theories of long-range and short-range interacting systems

The kinetic theory of systems with short-range interactions in the dilute gas limit involves the Boltzmann equation, a cornerstone of classical statistical mechanics (see, for example, Ref. [53] for a physical approach, or [54] for a precise mathematical discussion). Microscopically, particles travel at a typical velocity $\bar{v}$ and collide with each other after traveling a typical distance l, called the mean free path. Let σ be the diffusion cross-section for these collisions. One has $\sigma = \pi a^2$, where the parameter a is of the order of the particle radius. The mean free path is defined as $l = 1/\left(\pi a^2 n\right)$, where n is the typical particle density. The Boltzmann equation applies when the ratio $\Gamma = a/l$ is small (the Boltzmann–Grad limit [54]).

In the limit $\Gamma \to 0$, any two colliding particles can be considered as independent (uncorrelated) as they come from very distant areas. This is the basis of the Boltzmann hypothesis of molecular chaos (Stosszahl Ansatz). It explains why the evolution of the phase space distribution function $f(\mathbf{x}, \mathbf{p}, t)$ may be described by an autonomous equation, the Boltzmann equation, given by

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{\bar{v}}{l} C(f) . \tag{3}$$

Here m is the mass of the particles, while $C(f)$ represents collisional interactions between particles.

In what follows, we explain that, for systems with long-range interactions in the limit of large N, any two particles become statistically independent. This may seem paradoxical as, in this case, the force on every particle is the result of its interaction with all the other particles. The equivalent of the Stosszahl Ansatz (the fact that two particles are independent to leading order in $1/N$) here is then due to the law of large numbers: the force on each particle being the result of a large number of contributions from its interaction with all the other particles, the exact value of each contribution is of little importance and correlation between the motion of two particles is small. We explain this in more detail in Sections 2.2.2 and 2.2.3.

The analogy between the kinetic theory of dilute gases and that of systems with long-range interactions extend further. This is summarized in Table 1. The Boltzmann equation has a Lyapunov functional: the entropy, given by $-\int \mathrm{d}x\mathrm{d}p f \log f$, can be proven to increase in time (H-theorem). According to the classical argument, the entropy, $-\int \mathrm{d}x\mathrm{d}p f \log f$, is given by the number of microstates corresponding to the phase space distribution f, so long as two particles can be considered independent (this is the case in the Boltzmann–Grad limit). Moreover, it is a general property that, for a system in which the evolution of the macroscopic phase space density f is described by an autonomous equation, the number of microscopic states corresponding to f has to increase in time [55]. These two arguments thus explain why the H-theorem must hold for the Boltzmann equation. Since, for systems with long-range interactions, two particles can also be considered independent (see the previous paragraph), an H-theorem with the same entropy, given by $-\int \mathrm{d}x\mathrm{d}p f \log f$, must also hold in this case. The long-time evolution of systems with long-range interaction is governed by the Lenard–Balescu equation (Section 2.2.3), for which the entropy increase can actually be checked directly.

For the Boltzmann equation, there is an initial dynamical stage, independent of collisions, which is governed by the free transport only (Eq. (3), with the right hand side set to zero), and leads to local Poisson statistics [54]. Similarly, evolution of long-range interacting systems for short times leads to a state where two-point correlation functions are negligible, as

explained in Section 2.2.2. In short-range systems, when gradients of intensive parameters (density, temperature, etc.) are small, one achieves, for dilute gases, local thermodynamic equilibrium which is believed to hold in the limit of long times [54]. Similarly, systems with long-range interactions, on times of order one, converge towards "quasistationary states" (Section 2.2.2), which then evolve very slowly towards global statistical equilibrium (Section 2.2.3). Quasistationary states for long-range interacting systems are thus the analogue of local thermodynamic equilibrium of the Boltzmann equation for short-range systems.

Starting with Einstein's paper on Brownian motion, a very important class of works tries to relate macroscopic diffusion properties to microscopic correlations functions (Kubo-type formulae). An important result of classical kinetic theory is the long-time algebraic behavior of the correlation functions and Kubo integrands [56], and the related anomalous diffusion [56]. This leads to long-range temporal correlations of some statistical properties. As has been recently discovered, similar behavior occurs also in systems with long-range interactions [31–33]. We explain this in Section 2.2.5.

2.2.2. Vlasov dynamics and quasistationary states

We now derive heuristically the Vlasov equation from the Hamiltonian dynamics, Eq. (2). A particle with coordinate x feels a potential $V_{\text{discrete}}(x) = \frac{1}{N}\sum_i W(x - x_i)$. It is natural to consider the following continuum approximation to this potential:

$$V(x, t) = \int \mathrm{d}y\mathrm{d}p W(x - y) f(y, p, t). \tag{4}$$

The time evolution for the one-particle phase space distribution function $f(x, p, t)$ follows the Vlasov equation, given by

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} - \frac{\partial V}{\partial x}\frac{\partial f}{\partial p} = 0. \tag{5}$$

If $\{x_i\}$ were N independent random variables distributed according to the distribution f, Eq. (4) would then follow from the law of large numbers, and would be a good approximation to V_{discrete} up to corrections of order $1/\sqrt{N}$. Replacing the true discrete potential by V thus amounts to neglecting correlations between particles (the equivalent of the Stosszahl Ansatz) and finite-N effects. The potential V_{discrete} being replaced by an average one, namely, V, may be seen as a mean-field approximation to the dynamics.

That this approximation is valid in the limit $N \to \infty$ may be understood more precisely from a physical point of view in two different ways: by either writing the Bogoliubov–Born–Green–Kirkwood-Yvon (BBGKY) hierarchy, closing the hierarchy by considering a systematic expansion in powers of $1/N$, and keeping terms to leading order, or, by following the Klimontovich approach (see Section 2.2.3). The validity of the Vlasov equation has also been established with mathematical rigor for smooth W [57] (see also Ref. [54], and a more recent work, [58], for some classes of singular potential). These exact results show that the Vlasov equation is a good approximation to the particle dynamics, at least for times much smaller than $\log N$. Recent results showed that this $\log N$ is actually optimal, in the sense that there actually exist sets of initial conditions exhibiting divergence on times of order $\log N$ [59] (see an analogous $\log N$ timescale arising in Monte-Carlo dynamics for discrete spin systems considered in Section 2.3).

However, the "coincidence time" between the Vlasov dynamics and the Hamiltonian dynamics is generically much longer than $\log N$, meaning that most of the initial conditions have a "coincidence time" much longer than $\log N$. As will be discussed below, generic initial conditions converge towards a stable stationary state of the Vlasov equation on a timescale of order one, and then stay trapped close to this state for times algebraic in N (see Ref. [28] for a numerical observation and [60] for a mathematical investigation of the phenomenon).

As can be easily verified, the Vlasov equation, Eq. (5), inherits the conservation laws of the Hamiltonian dynamics, for instance, the energy

$$H[f] = \int \mathrm{d}x\mathrm{d}p \left[f\frac{p^2}{2} + \frac{fV[f]}{2} \right], \tag{6}$$

and the linear or the angular momentum when the system has the corresponding translational or rotational symmetry, respectively. The functionals,

$$C_s[f] = \int \mathrm{d}x\mathrm{d}p\, s(f(x, p, t)), \tag{7}$$

sometimes called Casimirs, are also invariant, *for any function s*.

Let us consider a dynamical system $\mathcal{F}$: $\dot{x} = F(x)$, with a conserved quantity $G(x)$ ($\dot{G}(x) = 0$). Any extremum x_0 of G represents an equilibrium of $\mathcal{F}$: $F(x_0) = 0$ and if, in addition, the second variations of G are either positive definite or negative definite, then this equilibrium is stable [61]. This general result seems natural if one considers the example of energy and angular momentum extrema encountered in classical mechanics. Then, as a consequence of the infinite number of conserved quantities, Eqs. (6)–(7), there exists an infinite number of equilibria f_0 for the Vlasov dynamics, a large number of them being stable [28]. In any dynamical system, fixed points play a major role. In the case of the Vlasov equation, they moreover turn out to be attractive, as illustrated by Landau damping [3]. Following these simple remarks, the following dynamical scenario was proposed [28]:

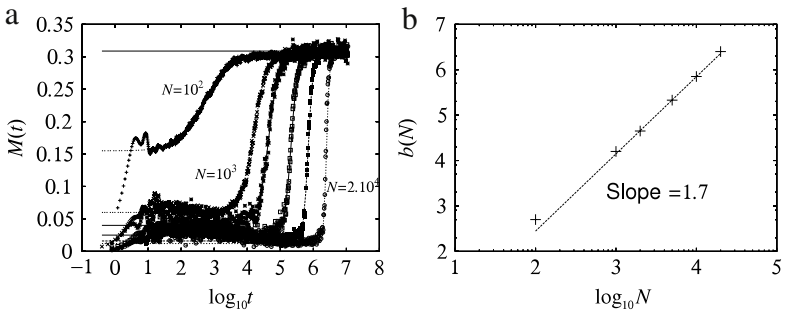

Fig. 4. Panel (a): Magnetization $M(t)$ of the HMF model, Eq. (8), for different particle numbers: from left to right, $N = 10^2$, 10^3, 2.10^3, 5.10^3, 10^4 and 2.10^4. The initial state is homogeneous in angles θ_i and uniform in momenta p_i. The horizontal line at the top represents the statistical equilibrium value of M. Panel (b) shows the logarithm of the relaxation timescale $b(N)$ as a function of $\ln N$, where the dashed line represents the law $10^{b(N)} \sim N^{1.7}$.
Source: The figure is taken from Ref. [28].

- Starting from some initial condition, the N-particle system approximately follows the Vlasov dynamics, and evolves on a timescale of order 1.
- It then approaches a stable stationary state of the Vlasov equation. Subsequently, the Vlasov evolution stops ("quasistationary states").
- Because of discreteness effects, the system evolves on a timescale of order N^α for some α, and slowly approaches the statistical equilibrium, moving along a series of stable stationary states of the Vlasov equation (see Section 2.2.3).

We note that a similar scenario was also observed in the plasma [3,30], astrophysical [29] and point vortex [5] contexts. As a concrete example, let us consider the case of the Hamiltonian mean-field (HMF) model, which involves classical XY spins with mean-field interactions [24]. Here the Hamiltonian is given by

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^{N} \left[1 - \cos\left(\theta_i - \theta_j\right)\right], \tag{8}$$

and the magnetization is given by $M = \left| \frac{1}{N} \sum_{i=1}^{N} \exp\left(\mathrm{i}\theta_i\right) \right|$. Note that, for the HMF model, the variables θ_i's play the role of the variables x_i's in the discussion following Eq. (2). For the HMF model, the above mentioned dynamical scenario is actually observed for initial states which are homogeneous in angles θ_i and uniform in momenta p_i (water-bag initial condition) [25,28] (see Fig. 4).

In this scenario, the N-particle system gets trapped for long times in out-of-equilibrium states close to stable stationary states of the Vlasov equation; these are called quasistationary states (QSS) in the literature. Before turning to a discussion of these states in the next paragraph, let us note that there is however no reason for this scenario to be the only possibility. For instance, the Vlasov dynamics could converge towards stable periodic solutions of the Vlasov equation [62].

We have explained that any Vlasov-stable stationary solution is a quasistationary state. Then, because inhomogeneous Vlasov-stationary states do exist, one should not expect quasistationary states to be homogeneous. This is illustrated in the case of several generalizations of the HMF model in [59].

The issue of the robustness of QSS when the Hamiltonian is perturbed by short-range interactions [50], or, when the system is coupled to an external bath [63] has also been addressed, and it was found that, while the power law behavior survives at least on some timescale, the exponent may not be universal. A possible statistical mechanical explanation of these QSS would be the "violent relaxation" theory of Lynden-Bell [8] and its generalizations. We refer to Ref. [6,64] and references therein for discussions on the interests and limitations of this approach.

2.2.3. Order parameter fluctuations and the Lenard–Balescu equation

In the previous subsection, we explained that, to leading order in $1/\sqrt{N}$, the dynamical evolution is described by the Vlasov equation. We now treat the $1/\sqrt{N}$ fluctuations of the order parameter, and the resulting correlations and corrections to the Vlasov equation. We assume that the initial condition is close to a QSS, and that this property holds in time as the system evolves (this is the equivalent of the propagation of local equilibrium for the Boltzman equation [54]).

In order to keep this discussion simple, we treat the case of the HMF model, Eq. (8). The case of a more general potential, Eq. (2), can be treated following exactly the same procedure. We follow [33], and refer to Ref. [53] for a plasma physics treatment, to Refs. [5,51,52] for the case of point vortices, and to Ref. [65] for self-gravitating stars.

A way to perform these computations would be an asymptotic expansion of the BBGKY hierarchy, where $1/\sqrt{N}$ is the small parameter (see, for instance, Ref. [3]). The $1/\sqrt{N}$ fluctuations would then be obtained by explicitly solving the dynamical equations for the two-point correlation function while truncating the BBGKY hierarchy by assuming a Gaussian closure for the three-point correlation function. Our presentation, giving the same results, rather follows the Klimontovich approach [3,53].

The state of the system of N particles can be described by the *discrete* single particle time-dependent density function $f_d(\theta, p, t)$, defined as $f_d(\theta, p, t) \equiv \frac{1}{N}\sum_{j=1}^{N} \delta\left(\theta - \theta_j(t)\right)\delta\left(p - p_j(t)\right)$, where δ is the Dirac delta function, (θ, p) the Eulerian coordinates of the phase space and (θ_j, p_j) the Lagrangian coordinates of the particles. By taking the time derivative of $f_d(\theta, p, t)$ and using Eq. (2), one finds that the dynamical evolution is described by the Klimontovich equation [3], given by

$$\frac{\partial f_d}{\partial t} + p\frac{\partial f_d}{\partial \theta} - \frac{\mathrm{d}V}{\mathrm{d}\theta}\frac{\partial f_d}{\partial p} = 0, \tag{9}$$

with

$$V(\theta, t) \equiv -\int_0^{2\pi} \mathrm{d}\theta' \int_{-\infty}^{\infty} \mathrm{d}p \cos(\theta - \theta') f_d(\theta', p, t). \tag{10}$$

Eq. (9) is the same as the Vlasov equation, Eq. (5) (with x replaced by θ). However, whereas Eq. (9) describes the evolution of a sum of Dirac distributions and is exact, the Vlasov equation describes a smooth distribution f understood as a local spatial average (or a temporal average, depending on the interpretation).

When N is large, it is natural to approximate the discrete density f_d by a continuous one, namely, $f(\theta, p, t)$. Considering an ensemble of microscopic initial conditions close to the same initial macroscopic state, one defines the statistical average $\langle f_d\rangle = f_0(\theta, p)$, while fluctuations are of order $1/\sqrt{N}$. We will assume that f_0 is any stable stationary solution of the Vlasov equation. The discrete time-dependent density function can thus be written as $f_d(\theta, p, t) = f_0(\theta, p) + \delta f(\theta, p, t)/\sqrt{N}$, where the fluctuation δf is of zero average. Similarly, we define the average potential $\langle V\rangle$ and its corresponding fluctuation $\delta V(\theta, t)$ so that $V(\theta, t) = \langle V\rangle + \delta V(\theta, t)/\sqrt{N}$. Inserting both expressions in the Klimontovich equation, Eq. (9), and taking the average, one obtains

$$\frac{\partial f_0}{\partial t} + p\frac{\partial f_0}{\partial \theta} - \frac{\mathrm{d}\langle V\rangle}{\mathrm{d}\theta}\frac{\partial f_0}{\partial p} = \frac{1}{N}\left\langle \frac{\mathrm{d}\delta V}{\mathrm{d}\theta}\frac{\partial \delta f}{\partial p}\right\rangle. \tag{11}$$

The above equation with the right hand side set to zero is the Vlasov equation. The exact kinetic equation, Eq. (11), suggests that the quasistationary states of Section 2.2.2 do not evolve on timescales much smaller than N; this explains the extremely slow relaxation of the system towards statistical equilibrium.

Let us now concentrate on stable homogeneous distributions $f_0(p)$. Then, one has $\langle V\rangle = 0$. Subtracting Eq. (11) from Eq. (9) and using $f_d = f_0 + \delta f/\sqrt{N}$, one gets

$$\frac{\partial \delta f}{\partial t} + p\frac{\partial \delta f}{\partial \theta} - \frac{\mathrm{d}\delta V}{\mathrm{d}\theta}\frac{\partial f_0}{\partial p} = \frac{1}{\sqrt{N}}\left[\frac{\mathrm{d}\delta V}{\mathrm{d}\theta}\frac{\partial \delta f}{\partial p} - \left\langle \frac{\mathrm{d}\delta V}{\mathrm{d}\theta}\frac{\partial \delta f}{\partial p}\right\rangle\right]. \tag{12}$$

For times much smaller than $\sqrt{N}$, we may drop the right hand side encompassing quadratic terms in the fluctuations. The fluctuating part δf is then described by the left hand side of Eq. (12), which is the linearized Vlasov equation.

The linearized Vlasov equation can be solved explicitly by introducing the spatio-temporal Fourier–Laplace transform of δf and δV. This leads to

$$\widetilde{\delta V}(\omega, k) = -\frac{\pi\left(\delta_{k,1} + \delta_{k,-1}\right)}{\varepsilon(\omega, k)}\int_{-\infty}^{+\infty} \mathrm{d}p\, \frac{\widetilde{\delta f}(0, k, p)}{\mathrm{i}(pk - \omega)}, \tag{13}$$

where the dielectric permittivity ϵ is given by

$$\epsilon(\omega, k) = 1 + \pi k\left(\delta_{k,1} + \delta_{k,-1}\right)\int_{-\infty}^{+\infty} \mathrm{d}p\, \frac{\frac{\partial f_0}{\partial p}}{(pk - \omega)}. \tag{14}$$

Eq. (13) describes exactly the fluctuations to leading order. From it, we can compute any quantity of interest, for instance, the potential autocorrelation or the right hand side of Eq. (11). We describe the results without reproducing here the computational details (which are long and tedious, see Refs. [33,53]).

Potential autocorrelation. For homogeneous states, by symmetry, one has $\langle\widetilde{\delta V}(\omega_1, k_1)\widetilde{\delta V}(\omega_2, k_2)\rangle = 0$, except when $k_1 = -k_2 = \pm 1$. For $k = \pm 1$, one gets, after a transient exponential decay, the general result

$$\langle \delta V(t_1, \pm 1)\delta V(t_2, \mp 1)\rangle = \frac{\pi}{2}\int_{\mathcal{C}} \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega(t_1 - t_2)}\frac{f_0(\omega)}{|\varepsilon(\omega, 1)|^2}. \tag{15}$$

This is an exact result to leading order.

Lenard–Balescu equation. In order to describe the slow evolution of the distribution f_0 due to finite-N effects, we evaluate the right hand side of Eq. (11) to order $1/N$. This is, for systems with long-range interactions, the analogue of the collision operator for the Boltzmann equation for dilute systems with short-range interactions. This collision operator is called the Lenard–Balescu operator and it leads to the Lenard–Balescu equation, given by

$$\frac{\partial f_0(p,t)}{\partial t} = -\frac{1}{N}\frac{\partial}{\partial p} LB[f],$$
$$LB[f] = \int \mathrm{d}p' \frac{1}{|\epsilon(1,1)|}\left(f_0(p)\frac{\partial f_0}{\partial p}(p') - f_0(p')\frac{\partial f_0}{\partial p}(p)\right)\delta(p-p'). \tag{16}$$

We have presented the computation of the Lenard–Balescu equation for the HMF model, where variables θ and p are one dimensional. The generalization of this computation to the general potential as in Eq. (2), and for variables $\mathbf{x}$ and $\mathbf{p}$ of dimensions larger than one leads to

$$\frac{\partial f_0(\mathbf{p},t)}{\partial t} = -\frac{1}{N}\frac{\partial}{\partial \mathbf{p}} LB[f], \tag{17}$$
$$LB[f] = \int \mathrm{d}\mathbf{k}\mathrm{d}\mathbf{p}' \frac{\phi(k)}{|\epsilon(k,\mathbf{k}.\mathbf{p}')|}\mathbf{k}.\left(f_0(\mathbf{p})\frac{\partial f_0}{\partial \mathbf{p}}(\mathbf{p}') - f_0(\mathbf{p}')\frac{\partial f_0}{\partial \mathbf{p}}(\mathbf{p})\right)\delta\left(\mathbf{k}.\left(\mathbf{p}-\mathbf{p}'\right)\right). \tag{18}$$

Here $\mathbf{k}$ is a wave vector, $\phi(k)$ is the Fourier transform of the potential $V(\mathbf{x})$, and $|\epsilon(k,\mathbf{k}.\mathbf{p}')|$ is the dielectric permittivity. We note that the Lenard–Balescu operator is a quadratic one, as is the collision operator $C(f)$ in the Boltzmann equation, Eq. (3). Moreover, this operator involves a resonance condition through the Dirac distribution $\delta\left(\mathbf{k}.\left(\mathbf{p}-\mathbf{p}'\right)\right)$.

From Eq. (16), we expect a relaxation towards equilibrium of any quasistationary state with a characteristic time of order N. We note that, for plasma or self-gravitating systems, due to the small distance divergence of the interaction potential, the Lenard–Balescu operator diverges at small scales. This is regularized by introducing a small scale cut-off. This leads to a logarithmic correction to the relaxation time, which is then the Chandrasekhar time for stellar systems, proportional to $N/\log N$.

One clearly finds from Eq. (16) that the mechanism for the evolution of the distribution function is related to two-particle resonances. An essential point is that the resonance condition $p - p' = 0$ cannot be fulfilled. This is because, with $p = p'$, the Lenard–Balescu operator, Eq. (16), which is odd in the variable p, would vanish.

For physical systems for which $\mathbf{x}$ is a one-dimensional variable, this proves that Vlasov-stable distribution functions do not evolve on timescales smaller or equal to N. This is an important result: *generic out-of-equilibrium distributions, for one-dimensional systems, evolve on timescales much larger than N* [66]. As noted in Ref. [33], this explains why for the HMF model, relaxation does not occur on times scales of order N (a $N^{1.7}$ scaling law was numerically observed in the HMF model [28], see Fig. 4, page 13). A similar kinetic blocking due to the same type of lack of resonances may also occur in the case of the point vortex model [67].

2.2.4. The stochastic process of a single particle

Let us now consider the relaxation properties of a test-particle, labeled by 1, surrounded by a background of $(N-1)$ particles with a homogeneous distribution $f_0(p)$. We want to describe the stochastic process of particle 1. We will first prove that the dynamics of this particle may be described by a Fokker–Planck equation. For this, we generalize the computations of Section 2.2.3. As in Section 2.2.3, for the sake of simplicity, we treat here the case of the HMF model, but extensions to the general case, Eq. (2), is straightforward.

We first compute the diffusion $\left\langle (p_1(t)-p_1(0))^2\right\rangle$, where $p_1(0)$ and $p_1(t)$ are the momentum of particle 1 at initial time and at time t, respectively. Here the brackets denote averaging over the initial positions and momenta of the remaining $N-1$ particles. Taking into account the knowledge of the position of particle 1, the distribution f_d (see Eq. (9)) is $f_d(\theta,p,t) = f_0(\theta,p) + \delta f(\theta,p,t)/\sqrt{N} + \delta(\theta-\theta_1, p-p_1)/N$, where δf is the zero-average fluctuation of the density of the remaining $N-1$ particles. We define the average potential $\langle V\rangle$ and its corresponding fluctuation $\delta V(\theta,t)$ so that $V(\theta,t) = \langle V\rangle + \delta V(\theta,t)/\sqrt{N}$. Then, from Eq. (10), we obtain

$$\delta V(\theta,t) = -\int_0^{2\pi}\mathrm{d}\theta' \int_{-\infty}^{+\infty}\mathrm{d}p\ \cos(\theta-\theta')\,\delta f(\theta',p,t) - \frac{1}{\sqrt{N}}\cos(\theta-\theta_1). \tag{19}$$

Using the equations of motion, Eq. (2), for the test particle and omitting from now on the label 1 for the sake of simplicity, one obtains

$$p(t) = p(0) - \frac{1}{\sqrt{N}}\int_0^t \mathrm{d}u \frac{\mathrm{d}\delta V}{\mathrm{d}\theta}(u,\theta(u)). \tag{20}$$

Then

$$\left\langle (p(t)-p(0))^2\right\rangle = \frac{1}{N}\int_0^t\int_0^t \mathrm{d}u\mathrm{d}u' \left\langle \frac{\mathrm{d}\delta V}{\mathrm{d}\theta}(u,x(0))\frac{\mathrm{d}\delta V}{\mathrm{d}\theta}(u',\theta(0))\right\rangle + \mathrm{O}\left(\frac{1}{N}\right). \tag{21}$$

In deriving the above equation, we have replaced $\theta(u)$ by $\theta(0)$ in Eq. (20), which is valid to leading order in $1/N$. From Eq. (19), it is clear that the average autocorrelation of the potential does not depend on particle 1 to leading order in $1/N$. Then, to leading order, Eq. (15) for the Laplace transform of the potential autocorrelation can be used. We obtain

$$\left\langle (p(t)-p(0))^2 \right\rangle \underset{t\to+\infty}{\sim} \frac{2t}{N} D(p), \tag{22}$$

where the diffusion coefficient $D(p)$ is explicitly computed from Eq. (15). One gets

$$D(p) = 2\,\mathrm{Re}\int_0^{+\infty} \mathrm{d}t e^{\mathrm{i}pt}\ \langle \delta V(t,1)\delta V(0,-1)\rangle = \frac{\pi^2 f_0(p)}{|\varepsilon(p,1)|^2}. \tag{23}$$

The computation of $\langle (p(t)-p(0))\rangle$ is less straightforward, as then the corrections to the potential due to particle 1 have to be evaluated to next order. These computations are not conceptually difficult (see Refs. [31–33]), but are too long to be presented here. We obtain

$$\langle (p(t)-p(0))\rangle \underset{t\to+\infty}{\sim} \frac{t}{N}\left(\frac{\mathrm{d}D(p)}{\mathrm{d}p} + \frac{1}{f_0}\frac{\partial f_0}{\partial p} D(p)\right). \tag{24}$$

As the changes in the momentum p are small (of order $1/\sqrt{N}$), the description of the stochastic process in momentum p by a Fokker–Planck equation is valid (see Ref. [68]). The Fokker–Planck equation is then characterized by the temporal behavior of the first two moments, $\left\langle (p(t)-p(0))^n \right\rangle$; $n=1,2$ [68]. Rescaling the time variable $\tau = t/N$, as suggested by Eqs. (24) and (22), the Fokker–Planck equation describing the time evolution of the distribution of the test particle is

$$\frac{\partial f_1(\tau,p)}{\partial \tau} = \frac{\partial}{\partial p}\left[D(p)\left(\frac{\partial f_1(\tau,p)}{\partial p} - \frac{1}{f_0}\frac{\partial f_0}{\partial p} f_1(\tau,p)\right)\right]. \tag{25}$$

We stress that this equation depends on the bath distribution f_0. It is valid for both equilibrium baths (Gaussian f_0) and out-of-equilibrium baths, provided that f_0 is a stable stationary solution of the Vlasov equation. It is easily checked that $f_1(p) = f_0(p)$ is the stationary solution to Eq. (25). Then, in the limit $\tau \to \infty$, the test particle probability density function f_1 converges towards the quasistationary distribution of the surrounding bath f_0. This is consistent with the result that f_0 is stationary for timescales of order N.

The Vlasov equation, the Lenard–Balescu equation and the Fokker–Planck equation for a test particle are all classical results. Recent results are the ones related to the understanding of the importance of QSS and their extensive study in the context of the HMF model. The Fokker–Planck diffusion coefficient has also been tested numerically [32]. In the next subsection, we explain other recent results related to the very interesting and peculiar properties of the Fokker–Planck equation, Eq. (25), and the associated algebraic temporal correlation and anomalous diffusion.

2.2.5. Long-range temporal correlations and anomalous diffusion

The quest for relations between observable macroscopic transport properties and microscopic properties are at the core of the program of equilibrium and out-of-equilibrium statistical mechanics. Historically, this has played an important role, not only from a practical point of view to have access to microscopic information without observing them directly, but also from a conceptual point of view. The Kubo-type formulae are an essential part of the theory, relating microscopic correlation functions to diffusion coefficients. In the 1970's, it came as a great surprise to discover that the integrand of the Kubo formulae may diverge and lead to anomalous diffusion and transport (see below). This led to a series of very interesting papers reviewed in Ref. [56].

We briefly recall that, when looking at the statistics of a spatial variable x as a function of time, when its moment of order n, $\langle x^n(\tau)\rangle$, scales like $\tau^{n/2}$ at long times, the associated transport is called *normal*. However, *anomalous* transport [69,70], where moments do not scale as in the normal case, is also known in some stochastic models, in continuous time random walks (Levy walks), in kinetic theory [56] and for systems with a lack of stationarity of the corresponding stochastic process [71].

In this subsection, we present recent results [33] that predicted the existence of non-exponential relaxation, autocorrelation of the momentum p with algebraic decay at long times, and anomalous diffusion of the spatial or angular variable x. These results thus show that, similar to the case of the classical theory of systems with short-range interactions [56], anomalous transport exists also in the kinetic theory of systems with long-range interactions. These results also clarify the highly debated disagreement between different numerical simulations reporting either anomalous [26] or normal [27] diffusion, in particular, by delimiting the time regime for which such anomalous behavior should occur. These theoretical predictions have been numerically checked in Ref. [72]. Some recent results, extending this work, have also been reported for the point vortex model [73]. We note that an alternative explanation, with which we disagree, both for the existence of QSS and for anomalous diffusion has been proposed in the context of Tsallis non-extensive statistical mechanics [74,75] (see Refs. [28,33,76] for further discussions).

Our results have been obtained by analyzing theoretically the properties of the Fokker–Planck equation, Eq. (25), derived in Section 2.2.4. From a physical point of view, as particles with large momenta p move very fast in comparison to the typical timescale of the fluctuations of the potential, they experience a very weak diffusion and thus maintain their large

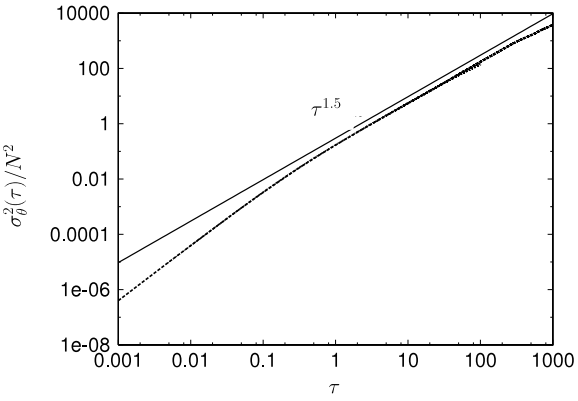

Fig. 5. Diffusion $(\sigma_\theta^2(\tau)/N^2 \equiv \left\langle(\theta(t)-\theta(0))^2\right\rangle/N^2$ as a function of time $\tau = t/N$) in the HMF model, for a quasistationary state. Points are from a N-body numerical simulation, the straight line is the analytic prediction by the kinetic theory. For long times, $\left\langle(\theta(t)-\theta(0))^2\right\rangle \sim_{t\to\infty} t^\nu$ with $\nu \neq 1$. A weak anomalous diffusion is also observed in equilibrium (see Ref. [33] for details).

Table 2
Theoretical predictions of the autocorrelation function $C_p(\tau)$ of the momentum p and of the standard deviation $\sigma_\theta^2(\tau)$ of the variable θ in the long-time regime, for different bath distributions $f_0(p)$. The results are valid for any bath distribution $f_0(p)$ which is strictly decreasing as $|p| \to \infty$, and depend on $f_0(p)$ only through its large p asymptotic behavior (tail of the distribution). The prediction for α is $\alpha = (\nu-3)/(\nu+2)$. See Fig. 5 for an illustration of these results using numerical simulations of the HMF model and Refs. [31,33] for more details.

Tails of the bath distribution function f_0	$f_0(p)$ $(\lvert p\rvert \to \infty)$	$C_p(\tau)$ $(\tau \to \infty)$	$\sigma_\theta^2(\tau)$ $(\tau \to \infty)$
Power-law	$\lvert p\rvert^{-\nu}$	$\tau^{-\alpha}$	$\tau^{2-\alpha}$
Stretched exponential	$\exp(-\beta\lvert p\rvert^\delta)$	$\frac{(\ln\tau)^{2/\delta}}{\tau}$	$\tau(\ln\tau)^{2/\delta+1}$

momentum during a very long time (one finds from Eq. (23), using $|\varepsilon(p,1)|^2 \to_{p\to\infty} 1$, that the diffusion coefficient decays as fast as the bath distribution $f_0(p)$ for large times). Because of this very weak diffusion for large p, the distribution of waiting time for passing from a large value of p to a typical value of p is a fat distribution. This explains the algebraic asymptotics for the correlation function. From a mathematical point of view, these behaviors are linked to the fact that the Fokker–Planck equation, Eq. (25), has a continuous spectrum down to its ground state (without gap). This leads to a non-exponential relaxation of different quantities and to long-range temporal correlations [31,33]. These results apply to the kinetic theory of any system for which the slow variable (here the momentum) lives in an infinite space. By explicitly deriving an asymptotic expansion of the eigenvalues and eigenfunctions of the Fokker–Planck equation, the exponent for the algebraic tail of the autocorrelation function of momentum has been theoretically computed [31,33]. The detailed analysis is a bit complex and tedious, thus, cannot be reproduced here (a detailed presentation can be found in Ref. [31]).

Let us present the results in the context of the HMF model, Eq. (8), for which algebraic long-time behavior for momentum autocorrelation has been first numerically observed in Refs. [74,75]. In its QSS, the theoretical law for the diffusion of angles $\sigma_\theta^2(\tau)$ has also been derived in Refs. [31,33]. The predictions for the diffusion properties are listed in Table 2 and illustrated using numerical simulations of the HMF model in Fig. 5.

When the distribution $f_0(p)$ is changed within the HMF model, a transition between weak anomalous diffusion (normal diffusion with logarithmic corrections) and strong anomalous diffusion is predicted (Table 2). We have numerically confirmed this theoretical prediction [72]. For initial distributions with power-law or Gaussian tails, correlation functions and diffusion are in good agreement with numerical results. Diffusion is indeed *anomalous super-diffusion* in the case of power-law tails, while *normal* when Gaussian. In the latter case, the system is in equilibrium, but the diffusion exponent shows a slow logarithmic convergence to unity due to a logarithmic correction to the correlation function. The long transient times before observing normal diffusion, even for Gaussian distribution and in equilibrium, suggests that one should be very careful to decide whether diffusion is anomalous or not from numerical simulations.

2.3. Dynamics of discrete spin systems

In this section, we discuss the relaxation process from a thermodynamically unstable state in long-range interacting systems with discrete degrees of freedom. These systems do not have intrinsic dynamics and one has to resort to Monte Carlo (MC) dynamics within either a microcanonical or a canonical ensemble. Here we briefly discuss the results for the Ising model with long- and short-range interactions, defined by the Hamiltonian in Eq. (1) [17].

Within a microcanonical ensemble, the dynamics followed in Ref. [17] is based on the microcanonical MC algorithm of Creutz [77]. In this algorithm, an extra degree of freedom, called the demon, with energy $E_D \geq 0$ samples microstates of the system with energy $E - E_D$ by attempting random single spin flips. At long times, to leading order in the system size N,

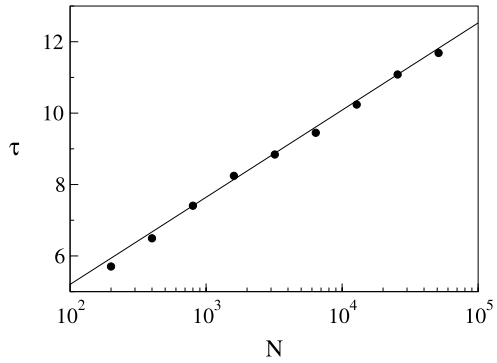

Fig. 6. Relaxation time of the $m = 0$ state when this is a local minimum of the entropy for the model in Eq. (1). Here $K = -0.25, J = 1, \epsilon = -0.2$.

the distribution of E_D attains the Boltzmann form, $P(E_D) \sim \exp(-E_D/k_BT)$, where T is the temperature of the system with energy E. As long as the entropy of the system increases with its energy, the temperature is positive and the average energy of the demon is finite and small compared with the system energy, with the latter scaling with N. The system energy at any given time is $E - E_D$, with finite fluctuations.

In applying the above dynamics to models with long-range interactions, one should note that, to next order in N, $P(E_D) \sim \exp(-E_D/T - E_D^2/2C_VT^2)$, where $C_V = O(N)$ is the system's specific heat. In systems with short-range interactions, the specific heat is non-negative so that the next-to-leading term in the distribution is a stabilizing factor which is negligible for large N. On the other hand, in systems with long-range interactions, C_V may be negative in some regions of the phase diagram, and on the face of it, the next-to-leading term may destabilize the distribution. However, the next-to-leading term is small, of $O(1/N)$, so that as long as the entropy increases with the energy, the next-to-leading term does not destabilize the distribution.

The above dynamics has been applied to the model in Eq. (1). It was found that, starting with a zero magnetization thermodynamically unstable state at energies where this state is a local minimum of the entropy, the model relaxes to the equilibrium, magnetically ordered state on a timescale which diverges with the system size as $\ln N$ (see Fig. 6).

To get insight into the above result for the relaxation time, we consider the Langevin equation corresponding to the dynamics, which is given by

$$\frac{\partial m}{\partial t} = \frac{\partial s}{\partial m} + \xi(t); \qquad \langle \xi(t)\xi(t')\rangle = D\delta(t - t'), \tag{26}$$

where $\xi(t)$ represents white noise. The diffusion constant D scales as $D \sim 1/N$. This may be seen by considering the non-interacting case in which the magnetization evolves by pure diffusion, where the diffusion constant scales in this form. Since we are interested in a thermodynamically unstable $m = 0$ state, corresponding to a local minimum of the entropy, we may, for simplicity, consider an entropy function of the form

$$s(m) = am^2 - bm^4, \tag{27}$$

with a and b non-negative parameters. The Fokker–Planck equation for the probability distribution $P(m, t)$ at time t reads

$$\frac{\partial P(m,t)}{\partial t} = D\frac{\partial^2 P(m,t)}{\partial m^2} - \frac{\partial}{\partial m}\left(\frac{\partial s}{\partial m}P(m,t)\right). \tag{28}$$

This equation may be viewed as describing the motion of an overdamped particle with coordinate m in a potential $-s(m)$ at a temperature $T = D$. To probe the relaxation process from the $m = 0$ state, it is sufficient to consider the entropy in Eq. (27) with $b = 0$. With the initial condition, $P(m, 0) = \delta(m)$, the long-time distribution is [78]

$$P(m,t) \sim \exp\left[-\frac{ae^{-at}m^2}{D}\right]. \tag{29}$$

It follows that the relaxation time from the unstable state, τ_{us}, which corresponds to the width reaching a value of $O(1)$, satisfies

$$\tau_{us} \sim -\ln D \sim \ln N. \tag{30}$$

Similar behavior has been found for the model in Eq. (1) with Metropolis-type canonical dynamics at fixed temperature [17]. Thus, the logarithmic divergence with N of the relaxation time seems to be independent of the nature of the dynamics (i.e., whether microcanonical or canonical).

The relaxation process from a metastable state (rather than an unstable state discussed above) has also been studied in the past [17]. Here the entropy has a local maximum at $m = 0$, while the global maximum occurs at some $m \neq 0$. As one

would naively expect, the relaxation time τ_{ms} from the metastable $m = 0$ state grows exponentially with N: $\tau_{ms} \sim e^{N\Delta s}$ [17]. The entropy barrier Δs corresponding to the non-magnetic state is the difference in entropy between that of the $m = 0$ state and the entropy at the local minimum separating it from the stable equilibrium state. Such exponentially long relaxation times are expected to occur independently of the nature of the order parameter or of the type of the dynamics (stochastic or deterministic). This has been found in the past in numerous studies of canonical, Metropolis-type dynamics, of the Ising model with mean-field interactions [79], in deterministic dynamics of the XY model [80], and in models of gravitational systems [81,82].

3. Weak long-range interactions

Here we consider systems with weak long-range interactions, with $\sigma > 0$. These systems are additive and thus, have usual properties as for systems with short-range interactions. This is true unless one is close to a phase transition, where, as mentioned in the Introduction, building up of long-range correlations leads to modification of the thermodynamic properties. For example, critical exponents near a continuous transition become dependent on the interaction parameter σ. In this Section, we briefly discuss the upper critical dimension $d_c(\sigma)$ for these systems above which the critical exponents assume the Landau or mean-field values. For details, see Ref. [83].

We first discuss the case of short-range interactions. We start with the coarse-grained Landau–Ginzburg effective Hamiltonian of the system. This Hamiltonian involves only the long-wavelength degrees of freedom, and is obtained by averaging over the short-wavelength ones. For a given system, one obtains this Hamiltonian phenomenologically from the symmetry properties of the order parameter involved in the transition. In systems with a single component, Ising-like order parameter, say, the magnetization, the effective Hamiltonian involves the local coarse-grained magnetization $m(\mathbf{r})$ defined at the spatial location $\mathbf{r}$. If the interaction is short-ranged, this Hamiltonian has the form

$$\beta H = \int d^d\mathbf{r}\left[\frac{1}{2}tm^2 + \frac{1}{4}um^4 + \frac{1}{2}(\nabla m)^2\right], \tag{31}$$

where t and $u > 0$ are phenomenological parameters, and d is the spatial dimension. Close to the critical temperature T_c, the parameter t may be taken to depend on temperature, $t \propto \frac{(T-T_c)}{T_c}$. Considering the model at $t > 0$, when the equilibrium state is a paramagnetic one, we first evaluate the fluctuations of the order parameter around its average value, $\langle m\rangle = 0$. Expressing the effective Hamiltonian in terms of the Fourier modes of the order parameter, $m(\mathbf{q}) = \int d^d\mathbf{r}e^{i\mathbf{q}\cdot\mathbf{r}}m(\mathbf{r})$, and neglecting the fourth-order term in Eq. (31) close to the transition, the Hamiltonian in the thermodynamic limit reduces to that of a Gaussian model. Thus, one has

$$\beta H = \frac{1}{2(2\pi)^d}\int d^d\mathbf{q}(t+q^2)m(\mathbf{q})m(-\mathbf{q}). \tag{32}$$

From this, it follows that the two-point correlation function, $\langle m(\mathbf{r})m(\mathbf{r}')\rangle$, is given by

$$\langle m(\mathbf{r})m(\mathbf{r}')\rangle = \frac{1}{(2\pi)^d}\int d^d\mathbf{q}\frac{e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}}{t+q^2}. \tag{33}$$

On scaling q by $\sqrt{t}$, the integral in Eq. (33) implies a correlation length $\xi = t^{1/2}$. At distances much larger than ξ, the correlation function decays exponentially as $e^{-|\mathbf{r}-\mathbf{r}'|/\xi}$, with a sub-leading power law correction.

From Eq. (33), integrating over modes with wavelengths bigger than the correlation length ξ, one gets

$$\langle m^2(\mathbf{r})\rangle = \int_{q<\sqrt{t}}\frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{t+q^2} \propto t^{\frac{d}{2}-1}. \tag{34}$$

In the Landau or mean-field theory, one neglects fluctuations of the order parameter. To find the dimensions at which this assumption is valid, let us first consider the fluctuations of the order parameter about its average below the critical point ($t < 0$) by writing $m(\mathbf{r})$ as $m(\mathbf{r}) = m_0 + \delta m(\mathbf{r})$, where the average $m_0 = \sqrt{-\frac{t}{u}}$. With this form for $m(\mathbf{r})$, from Eq. (31), it follows that, to second order in $\delta m(\mathbf{r})$, the Landau–Ginzburg effective Hamiltonian close to the transition point is given by

$$\beta H = \int d^d\mathbf{r}\left[\frac{1}{2}|t|(\delta m(\mathbf{r}))^2 + \frac{1}{2}(\nabla\delta m(\mathbf{r}))^2\right]. \tag{35}$$

We now see that the fluctuations of the order parameter around the average value below but close to the transition obey a Hamiltonian similar to that for the fluctuations above and close to the transition. It then follows from Eq. (34) that $\langle\delta m^2(\mathbf{r})\rangle \propto |t|^{\frac{d}{2}-1}$. For the Landau theory to be self-consistent near the transition, fluctuations of the order parameter should be negligibly small compared with the average value of the order parameter, $\langle\delta m^2(\mathbf{r})\rangle \ll m_0^2$, which is true so long as d is greater than the upper critical dimension $d_c = 4$. In dimensions less than 4, negligible fluctuations of the order parameter around its average can be achieved only away from the critical point for $|t| > |t_G|$, where t_G defines the Ginzburg temperature interval. This is known as the Ginzburg criterion [84–86].

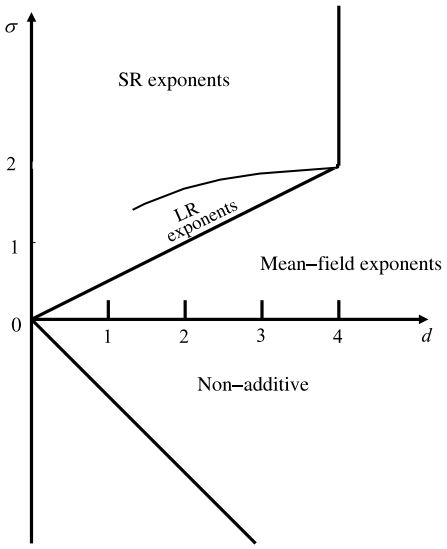

Fig. 7. The schematic (d, σ) phase diagram, showing various regions with different critical behavior. Here LR stands for long-range, while SR stands for short-range. The system is non-additive with strong long-range interactions for $d \leq \sigma \leq 0$. For $\sigma > 0$, the critical exponents can be either mean-field like, short-range like or characteristic of the long-range interactions, depending on σ and d. The line separating the LR from the SR behavior is indicated close to the point $d = 2\sigma = 4$, where it has been evaluated using Renormalization Group calculations in $d = 2\sigma - \epsilon$ dimensions. Note that for the case $\sigma > 2$, no phase transition takes place for $d \leq 1$.

Extending this analysis to systems with weak LRI, one finds that the Landau–Ginzburg effective Hamiltonian takes the form

$$\beta H = \int d^d\mathbf{r} \left[\frac{1}{2}tm^2 + \frac{1}{4}um^4\right] + \int d^d\mathbf{r}\, d^d\mathbf{r}' m(\mathbf{r})m(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|^{d+\sigma}}, \tag{36}$$

where the second integral accounts for the contribution from the long-range interaction potential to the energy. Next, we note that, to leading order in q, the Fourier transform of the long-range potential is of the form $a + bq^\sigma$, where a and b are constants (For integral σ, a logarithmic correction is present, e.g., $a + bq^2 \ln q$ for $\sigma = 2$; however, these logarithmic corrections do not affect the conclusions reached below.). In terms of the Fourier components of the order parameter, the Landau–Ginzburg effective Hamiltonian close to the transition thus takes the form

$$\beta H = \frac{1}{2(2\pi)^d} \int d^d\mathbf{q} (\bar{t} + bq^\sigma + q^2) m(\mathbf{q}) m(-\mathbf{q}), \tag{37}$$

where $\bar{t} = t + a$.

To obtain the upper critical dimension, one may now perform an analysis similar to that discussed above for systems with short-range interactions. For $\sigma > 2$, the q^σ term in Eq. (37) may be neglected in comparison to the q^2 term. One then recovers the behavior for models with short-range interactions and the upper critical dimension is $d_c = 4$. On the other hand, for $0 < \sigma < 2$, the dominant term is q^σ. The correlation length in this case diverges as $\xi \propto |\bar{t}|^{-1/\sigma}$. The order parameter fluctuations satisfy

$$\langle (\delta m(\mathbf{r}))^2 \rangle = \int_{q<1/\xi} \frac{d^d\mathbf{q}}{(2\pi)^d} \frac{1}{|\bar{t}| + q^\sigma} \propto |\bar{t}|^{d/\sigma - 1}. \tag{38}$$

Requiring that the fluctuations are much smaller than the average value of the order parameter $m_0 = \sqrt{-\frac{\bar{t}}{u}}$, one concludes that the upper critical dimension is $d_c = 2\sigma$. Thus, in $d < 4$ dimensions, there exists a critical σ, given by $\sigma_c(d) = \frac{d}{2}$, such that, for $0 < \sigma < \sigma_c(d)$, the critical exponents are mean-field like.This naive approach suggests that, for $\sigma_c(d) < \sigma < 2$, the critical exponents are affected by the long-range nature of the interaction and hence, become dependent on σ, see Ref. [38]. In fact, it has been shown using Renormalization Group in $d = 2\sigma - \epsilon$ dimensions that the value of σ above which short-range behavior is recovered is smaller than 2, and depends on the dimension d [87].

These conclusions are schematically shown in Fig. 7, where the associated critical behavior in different regimes are also indicated.

4. Nonequilibrium steady states and long-range interactions

We now turn to discuss steady states in systems driven out of equilibrium. In these systems, the drive may be provided either by an external force, such as due to an electric field, or by coupling to external thermostats at different temperatures.

We consider here systems for which the dynamics is conserving and local. These systems are typically characterized by long-range correlations which have been shown to lead to phase transitions and long-range order in many one-dimensional models. For reviews on steady state properties of driven models, see, for example, Refs. [88–91]. In some models, features characteristic of strong LRI, such as inequivalence of ensembles, have been observed [92]. In this Section, we discuss a particular model with local dynamics, called the *ABC* model, which exhibits spontaneous symmetry breaking in one dimension and for which such correlations can be explicitly demonstrated [42,43]. Moreover, for particular values of the parameters defining this model, the steady state becomes an equilibrium state obeying detailed balance. The weights of configurations in such a state are given by an effective Hamiltonian, which has explicit long-range interacting terms.

The model is defined on a one-dimensional lattice of N sites with periodic boundary conditions. Each site is occupied by either an A, a B, or a C particle. Configurations evolve by random sequential dynamics as follows: at each time step, two neighboring sites are chosen randomly and the particles on these sites are exchanged according to the following rules:

$$\begin{aligned} AB &\underset{1}{\overset{q}{\rightleftarrows}} BA \\ BC &\underset{1}{\overset{q}{\rightleftarrows}} CB \\ CA &\underset{1}{\overset{q}{\rightleftarrows}} AC. \end{aligned} \tag{39}$$

The rates are cyclic in A, B and C and conserve the total number of particles N_A, N_B and N_C of each type, respectively.

For $q = 1$, the particles undergo symmetric diffusion. At long times, the system reaches an equilibrium steady state, which is disordered. However, for $q \neq 1$, the particle exchange rates are biased, and the system settles into a nonequilibrium steady state which shows separation of the particle species into three distinct domains in the thermodynamic limit.

To be specific, we take $q < 1$, although the analysis is easily extended to any $q \neq 1$. In this case, the bias drives, say, an A particle to move to the left inside a B domain, and to the right inside a C domain. Therefore, starting with a random initial configuration, after a relatively short time, the system reaches a configuration of the type $\ldots AABBCCAAAB \ldots$ in which A, B and C domains are located to the right of C, A and B domains, respectively. Due to the bias $q < 1$, the domain walls $\ldots AB \ldots$, $\ldots BC \ldots$, and $\ldots CA \ldots$, are stable, and configurations of this type are long-lived. In fact, the domains in these configurations diffuse into each other and coarsen on a timescale of the order of q^{-l}, where l is the typical domain size. This coarsening process leads to the growth of the typical domain size as $(\ln t)/|\ln q|$. Eventually, the system settles into a phase-separated state of the form $A \ldots AB \ldots BC \ldots C$. A finite system does not stay in such a state indefinitely. For example, the A domain breaks up into smaller domains in a time of order $q^{-\min\{N_B, N_C\}}$. In the thermodynamic limit, however, when the density of each type of particles is non-vanishing, the timescale for the break up of extensive domains diverges and the system remains in the phase-separated state forever. Generically, the system supports particle currents in the steady state. This can be seen by considering, say, the A domain in the phase-separated state. The rates at which an A particle traverses a B (C) domain to the right (left) is of the order of q^{N_B} (q^{N_C}), so that the net current is of order $q^{N_B} - q^{N_C}$, vanishing exponentially with N. This implies that, for the special case of equal densities of the three particle species, $N_A = N_B = N_C$, the current is zero for any system size.

One finds that, for the special case of equal densities, $N_A = N_B = N_C$, the dynamics satisfy *detailed balance* with respect to a distribution function. The model in this case reaches an equilibrium steady state. It turns out however that, although the dynamical rules of the model are *local*, the effective Hamiltonian corresponding to this equilibrium steady state has *long-range interactions*, and thus, supports phase separation, consistent with our predictions above.

In order to specify the probability distribution of configurations for equal densities, we define a local occupation variable $\{X_i\} = \{A_i, B_i, C_i\}$, where A_i, B_i and C_i are equal to one if site i is occupied by an A, a B, or a C particle, respectively, and is zero otherwise. The probability of finding the system in a configuration $\{X_i\}$ is given by

$$W_N(\{X_i\}) = Z_N^{-1} q^{H(\{X_i\})}, \tag{40}$$

where the effective Hamiltonian H is given by

$$H(\{X_i\}) = \sum_{i=1}^{N-1} \sum_{k=i+1}^{N} (C_i B_k + A_i C_k + B_i A_k) - (N/3)^2, \tag{41}$$

and the normalization or the partition function Z_N is given by $Z_N = \sum q^{H(\{X_i\})}$. In this Hamiltonian, the site $i = 1$ is arbitrary and can be chosen as any other site on the ring, since the Hamiltonian does not depend on this choice. The Hamiltonian involves strong long-range interactions, where the strength of the interaction between two sites is independent of the separation (thus, $\sigma = -1$). Also, the Hamiltonian is non-extensive, with energy scaling as N^2. It may be verified that the dynamics (39) satisfy detailed balance with respect to the probability distribution in Eq. (40), with the Hamiltonian in Eq. (41) [83].

The *ABC* model exhibits phase separation and long-range order so long as $q \neq 1$. The parameter q acts like the temperature for the case of equal densities, with $\beta = -\ln q$, as can be seen from Eq. (40). A very interesting limit is that of infinite temperature, with $q \to 1$. To probe this limit, Clincy and co-workers [93] studied the case $q = \mathrm{e}^{-\beta/N}$, which

amounts to either scaling the temperature by N, or, alternatively, scaling the Hamiltonian in Eq. (41) by $1/N$, as is done in the prescription due to Kac (Section 2.1). In this case, the model shows a phase transition from a homogeneous phase at high temperatures to a phase-separated one at low temperatures across the critical point $\beta_c = 2\pi\sqrt{3}$.

In this section, we discussed how, in the *ABC* model for equal particle densities, the effective Hamiltonian governing the steady state involves explicitly strong long-range (in fact, mean-field) interacting terms. By continuity, this is expected to hold even for the case of non-equal densities, although, in such cases, no effective Hamiltonian could be explicitly written. It remains to explore in more detail steady state properties of driven systems within the framework of systems with long-range interactions.

5. Conclusions

In this paper, we reviewed the thermodynamic and dynamic properties of systems with long-range pairwise interactions (LPI) decaying as $1/r^{d+\sigma}$ at large distances r in d dimensions. Systems with a slow decay of the interactions, termed "strong" LRI, have superextensive energy. These systems are characterized by unusual properties such as inequivalence of ensembles, negative specific heat, slow decay of correlations, anomalous diffusion and ergodicity breaking. Systems with faster decay of the interaction potential, termed weak "LRI", have additive energy, thus resulting in less dramatic effects. These interactions affect the thermodynamic behavior of systems near phase transitions, where long-range correlations are naturally present. We also discussed long-range correlations in systems driven out of equilibrium when the dynamics involves conserved quantities.

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