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Microscopic reversibility and macroscopic irreversibility: A lattice gas model

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HIGHLIGHTS

- The transition from microscopic reversibility to macroscopic irreversibility.
- Reversible and recurrent behavior is tied to deterministic rules of motion.
- Irreversible behavior arises from the introduction of probabilistic considerations.

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ABSTRACT

We present coarse-grained descriptions and computations of the time evolution of a lattice gas system of indistinguishable particles, whose microscopic laws of motion are exactly reversible, in order to investigate how or what kind of macroscopically irreversible behavior may eventually arise. With increasing coarse-graining and number of particles, relative fluctuations of entropy rapidly decrease and apparently irreversible behavior unfolds. Although that behavior becomes typical in those limits and within a certain range, it is never absolutely irreversible for any individual system with specific initial conditions. Irreversible behavior may arise in various ways. We illustrate one possibility by replacing detailed integer occupation numbers at lattice sites with particle probability densities that evolve diffusively.

1. Introduction

Thermodynamic descriptions of the approach to equilibrium for macroscopic systems are typically irreversible, whereas classical or quantum descriptions of motion of their microscopic constituents are typically reversible. Reconciling these views is still a matter of inquiry.

In a macroscopic thermodynamic framework, we may characterize a system in terms of just a few macroscopic variables, whereas in an underlying microscopic approach we must typically consider a vastly greater number of degrees of freedom, such as those accounting for velocities and positions of all particles in the system.

A ground-breaking connection between microscopic and macroscopic viewpoints was established by Boltzmann in an 1872 paper, where he derived his celebrated transport equation and his consequent H-theorem [1–9]. That theorem provided a microscopic insight on how prototypical physical systems with a large number of particles exhibit a natural tendency to evolve towards definite states of macroscopic equilibrium. The H-theorem also demonstrated how a system,

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after attaining a state of macroscopic equilibrium, tends to remain in that macroscopic state almost indefinitely, if left undisturbed.

From the beginning, Boltzmann's revolutionary ideas were fiercely debated [6–9]. Major developments in statistical and quantum theories have since vastly broadened, but invariably confirmed, the scope and validity of Boltzmann's ideas. Still, the original question remains: how or when can macroscopic irreversibility ultimately arise from microscopic reversibility, either in theory or in practice? Boltzmann's H-theorem applied specifically to dilute gases and he arrived at its conclusion by introducing a probabilistic element, known as 'Stosszahlansatz', or the assumption of 'molecular chaos', which constrains the manner in which particles may exchange momentum through collisions. Based on that microscopic assumption, the H-theorem describes a thermodynamic evolution of entropy towards a most probable macroscopic state of equilibrium [1–9].

Those who initially objected to Boltzmann's ideas did so on the basis of two major difficulties. The first, introduced by Thomson (1874) and Loschmidt (1876), arises from the apparent incompatibility between the time-reversal symmetry of the laws of motion applied to atoms and molecules and the characteristic irreversibility of macroscopic thermodynamics. This leads to the so called '*arrow-of-time dilemma*', whose possible origins have ever since been extensively debated and broadened [10]. The second difficulty, originally stressed by Zermelo (1896), refers to Poincaré's recurrence theorem (1890), stating that ''any phase-space configuration (q, p) of a system *enclosed in a finite volume* will be repeated as accurately as one wishes after a finite (be it possibly very long) interval of time'', which has become known as the *recurrence time* or a *Poincaré cycle* [11]. Quantum mechanical versions of the recurrence theorem have been subsequently derived [12–14].

Under certain conditions, which are technically specified as the Boltzmann–Grad limit, Lanford has been able to derive rigorously the irreversible Boltzmann transport equation from the reversible Hamiltonian dynamics of a system of hard spheres, or more generally for finite range interactions. His technique and results are presently limited to very short times, and apply to typical microscopic phase-space states with respect to a suitable measure [7].

Some rigorous results in the statistical treatment of the quantum mechanical evolution of complex multi-particle systems towards various states of equilibrium have been recently derived [15,16]. Such remarkable theoretical progress has been inspired or supported by computational models [17–19].

Questions of microscopic reversibility vs. macroscopic irreversibility are still subject to fundamental inquiry [20–23]. Technological advances allow such issues to be probed at increasingly deeper levels of microscopic dynamics [24,25]. Recent and future developments are expected to advance our understanding of relations between microscopic and macroscopic laws of motion and corresponding time evolutions of both 'simple' and 'complex' systems [26].

A formal discussion of reversible-to-irreversible transitions that may arise in complex systems with a large number of degrees of freedom is beyond the scope of this paper. Instead, we consider, mainly from a numerical perspective, a discrete model that simply illustrates certain features of reversible-to-irreversible transitions.

2. A lattice gas system

The two-dimensional system that we consider is a well-known square-lattice gas model originally introduced by Hardy, Pomeau and de Pazzis (HPP) [27,28]. It consists of *indistinguishable* particles that can occupy only the sites or nodes of a square lattice, with velocities of equal magnitude that can have only lattice directions, i.e., up, right, down, and left. Furthermore, no two particles are allowed to have the same velocity direction at the same site. Figs. 1a and 1b show a lattice gas example, where particles are represented by arrows, indicating their velocity directions. Like space and direction, time is also discretized. In each *time unit*, the particle dynamics is determined by two consecutive steps:

(1) *Translation step*: Each particle jumps to an adjacent site according to its velocity direction—see Fig. 1a and 1b. If a particle reaches an edge of the system, then its velocity direction is rotated by 180° at that time.
(2) *Interaction step*: No rotation of velocity direction occurs otherwise, except in the following case. When just two particles (and no more) enter the same site with opposite directions, their directions are rotated by 90°, while still maintaining opposite directions. Particles thus become *indistinguishable*, because there is no way to determine which particle rotated by 90° to its right or to its left. The computational algorithm implementing this rule is more explicitly described in Appendix A.

The system evolves *deterministically* and *reversibly* in time by application of those two simple rules. For example, in Fig. 1a we show a region of a lattice gas system at time $t = t'$, where sites are identified by their Cartesian coordinates and particles are represented by arrows indicating their directions. For example, site (6, 6) is maximally occupied with four particles. At the subsequent time $t = t' + 1$, after one *translation* and one *interaction* step, the system evolves to the configuration shown in Fig. 1b. Notice, for example, that although particles **a**, **b**, and **c** have met at site (5, 5), they were not allowed to interact, hence they have all maintained their identity and direction. Conversely, particles **e** and **f**, observed at $t = t'$ in Fig. 1a, meet all by themselves at site (6, 7) at $t = t' + 1$ in Fig. 1b: they must then rotate their directions by 90°, while still maintaining opposite directions. These two particles must now be re-labeled with different symbols, e.g., **u** and **v** in Fig. 1b, because our rules prevent the identification of each individual particle just after it has been involved in a 90° rotation, which could have been either to its right or to its left. Particles thus become *indistinguishable* on that account, as demonstrated algorithmically in Appendix A.

The rules of motion of our simple system mimic rudiments of the microscopic dynamics obeyed by atoms or molecules in a dilute fluid. Basically, these microscopic rules and laws are *deterministic*, *reversible*, and applicable to *indistinguishable*