Unpredictability of symmetry breaking in a phase transition

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We study the sensitive dependence on initial conditions of the final states of systems undergoing a symmetry-breaking phase transition. If the knowledge of the initial state is incomplete the macroscopic final state is unpredictable. This is demonstrated by computer simulations for two simple classical many-body systems. Next, this unpredictability is discussed within the more general framework of quantum field theories. For infinite systems a mixing property is exposed that prevents long-time predictions on the basis of local measurements. Finally, we remark on the more philosophical question whether the symmetry breaking of a highly symmetric theory after the big bang can be predicted or has to be considered as an historical accident.

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I. INTRODUCTION

The laws of physics as we see them today are supposed to be the result of a phase transition which happened shortly after the big bang. Thereby a highly symmetric unified theory ("theory of everything," TOE) was broken down into the various interactions we find now. They are all assumed to be contained in the TOE and, in principle, derivable from it. In this paper we shall investigate to what extent the outcome of a symmetry breaking in a phase transition can be predicted. Although the TOE is presumably deterministic one is dealing with a system of many particles (10^{88} at present) where not everything can be measured. Thus we shall investigate *how much the outcome of a phase transition is influenced by the fact that the initial state contains elements which are not completely determined.*

In Sec. II we shall do this first by studying two classical models. One is a system of 400 particles with attractive two-body potentials, the other is a 100×100 spin system on a lattice with ferromagnetic interactions. In both examples we work in an energy range where theory predicts a phase transition to occur and, indeed, practically for all initial conditions sooner or later a phase transition takes place. In both cases it breaks the symmetry of the system. In the first case a cluster is formed breaking the translational symmetry, in the second case the up-down symmetry is broken. In both cases the outcome of the phase transition (position of the cluster or direction of the spins) shows exceedingly sensitive dependence on initial conditions. We demonstrate that if we leave the initial conditions for all but two particles (or spins) the same and for those two we just interchange part of their initial data the resulting pattern of symmetry breaking is completely different.

After these computer solutions of simple classical many-body systems with deterministic and time-reversible equations of motion we turn in Sec. III to a theoretical study of unpredictability in the quantum theory of large systems. So far relativistic quantum field theories give the best framework for a TOE and there the situation is analogous to our classical models: What one can measure are only local quantities and there always remains an unobserved outer part; These theories presumably have a property which is called mixing and this tells us that in spite of the deterministic time evolution long-term predictions become impossible.
These results suggest to us that although a TOE may contain all the known laws of nature and many other possible laws as potentiality our present situation is the result of historical accidents which are beyond the predictive power of any kind of theory known today.

II. TWO EXAMPLES FROM CLASSICAL MECHANICS

Our arguments are based on the assumption of a very sensitive initial-condition dependence of the final states of a system undergoing a symmetry-breaking phase transition. We want to illustrate this point by two examples taken from classical mechanics.

A. Translational symmetry breaking in self-gravitating systems

A many-body system of particles interacting with purely attractive forces is known to be mechanically and thermodynamically unstable if its energy is below a certain threshold [1,2]. Computer simulations reveal that—even if one starts out with initial conditions for the particles homogeneous in space [Fig. 1(a)] and with a Maxwell-Boltzmann distribution in momentum space—clusters are formed very quickly which float in the rest-atmosphere of the remaining particles [Fig. 1(b)]. For this qualitative behavior the precise shape of the attractive pair potential and the dimension of space is immaterial. Our example is for a two-dimensional system of

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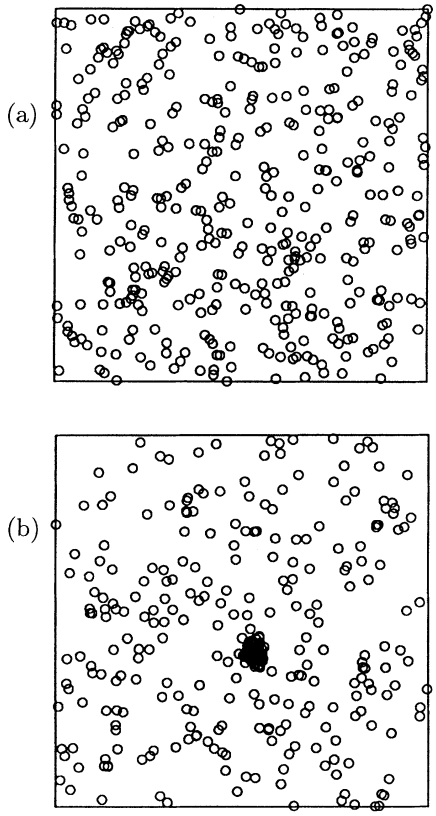

FIG. 1. (a) and (b) Snapshots of the homogeneous random initial configuration (a) and of a final clustered state (b) for the planar 400-particle system of Sec. II A. In reduced units the volume $V = 800$, and the particle diameter in the figure is $1/\sqrt{2}$, the inflection point of the attractive potential.

$N = 400$ particles confined to a square volume V with periodic boundary conditions, for which the Hamiltonian is written as

$$H_N = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i(<j)} \sum_{j} v(\mathbf{x}_i - \mathbf{x}_j).$$

Here, $\mathbf{x_i}$ and $\mathbf{p_i}$ denote the position and momentum of particle i, and m is the mass taken to be equal for all particles. For the pair potential we take a short-ranged negative Gaussian,

$$v(\mathbf{x} - \mathbf{y}) = -\kappa \exp[-(\mathbf{y} - \mathbf{x})^2/\sigma^2].$$

With this choice the singularity at the origin and the long-range cutoff problems inherent to the gravitational $1/x$ potential are avoided in the simulation, but the essential instability properties of gravitational systems are retained. Extensive computer simulations have been carried out with this model [3–6] which has interesting equilibrium properties (such as a negative specific heat in a certain range of energies) and a pronounced transient dynamical behavior while approaching equilibrium. For a finite volume V the collapsed equilibrium state is characterized by a *single* cluster which may contain a sizable fraction of all particles [$N_c \sim 2N/\ln(V/\sigma^2)$], and which performs a Brownian motion in the gas of the remaining particles as depicted in Fig. 2(a). This cluster is formed very early in the simulation run by acquiring more and more particles from the gas. During that transient growth it also heats up considerably [4] with a kinetic temperature $T \equiv K_c/N_c \sim N_c$, where K_c is the peculiar kinetic energy of the cluster particles. If reduced units are used for which the potential parameters κ, σ and the

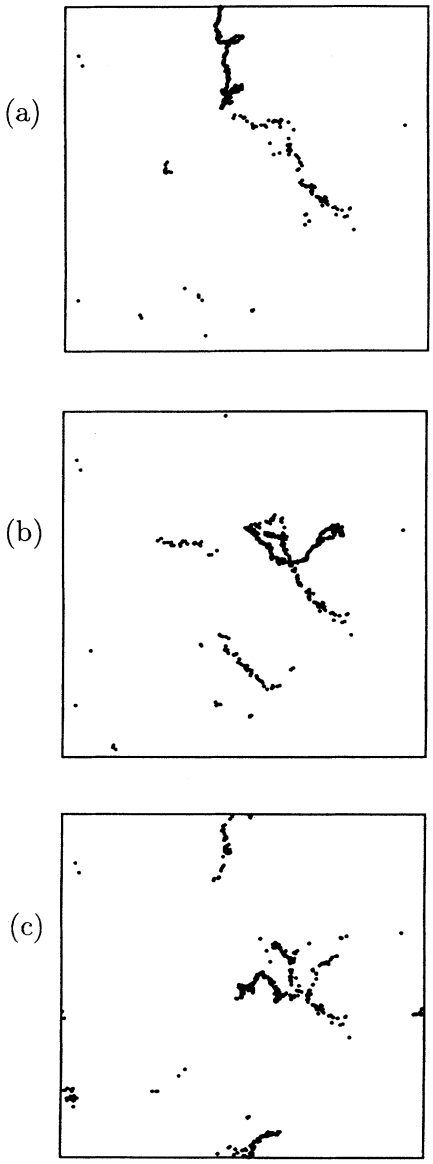

FIG. 2. (a)–(c) Instantaneous location of the center of mass of the largest cluster formed during the first 100 time units of a simulation run for the 400-particle model of Sec. II A. (a) reference system; (b) the x components of the momenta in the initial conditions of two particles are interchanged. (c) The y components of the momenta in the initial conditions of two particles are interchanged.

mass m are unity, the time required to reach the equilibrium cluster size is of the order of $t \sim 40$, although it takes at least 200 times longer to reach thermal equilibrium between the cluster and the surrounding gas [4]. In Fig. 2(a) the points indicate the Brownian motion of the center of mass of the largest cluster during the first 100 time units of the simulation run.

The homogeneous initial state [Fig. 1(a)] is translationally invariant. However, this symmetry is broken in the early stages of the phase transition by the formation of the main cluster, but the exact location where this cluster is formed depends very sensitively on the initial conditions. To demonstrate this fact the simulation leading to Fig. 2(a) was repeated with identical initial conditions with the exception of two particles for which the x components of their momenta were interchanged. This slight modification also leaves the total energy and momentum unaffected. The result is shown in Fig. 2(b). An analogous interchange of the y components of the momenta of the same pair of particles leads to Fig. 2(c). It is obvious that there is no resemblence between these three pictures as a result of the Lyapunov instability of the system in spite of the very weak perturbation applied to the initial state. Any slight ignorance about the initial state is dramatically amplified by the symmetry-breaking phase transition and leads to different macroscopic final states.

Even in low-dimensional systems with more than one attractor competing with each other and with a fractal boundary between their respective basins of attraction, a similar sensitive dependence of the occupancy of the final attractors on initial conditions has been found [7,8].

B. Dynamics of phase transition in a two-dimensional Ising model

The second example we want to consider is a deterministic Ising spin system in two dimensions exhibiting a ferromagnetic phase transition [9]. This algorithm is based on a deterministic cellular automaton rule. It is *invariant with respect to time reversal* and exactly conserves the total energy

$$H = -J \sum_{\{i,j\}} s_i s_j + \sum_i K_i .$$

The first term in this equation is the usual ferromagnetic ($J > 0$) Ising energy with spins $s_i \in \{+1, -1\}$ on site i, and the sum is over all next-neighbor pairs of lattice sites. The second term is the kinetic-energy where $K_i \in \{0, 4J, 8J, 12J\}$ is the kinetic-energy contribution of site i and may be associated with a momentum variable conjugate to spin s_i. Using periodic boundaries, any spin s_i is surrounded by four next neighbors. If it is flipped the Ising energy changes by a multiple of $4J$. This move will be accepted only if the kinetic-energy variable K_i can be varied accordingly to keep the total energy a constant. If the change of the Ising energy cannot be absorbed by K_i the move is not accepted and s_i, K_i remain unchanged. Checkerboard updating is used for all sites [9] such that in a first sweep through the system black sublattice sites are updated first with the white sublattice sites left unchanged. In a second sweep the role of the black and white sublattices is exchanged. A full time step requires an update of all sites and consequently two consecutive sweeps through the system. Since the kinetic

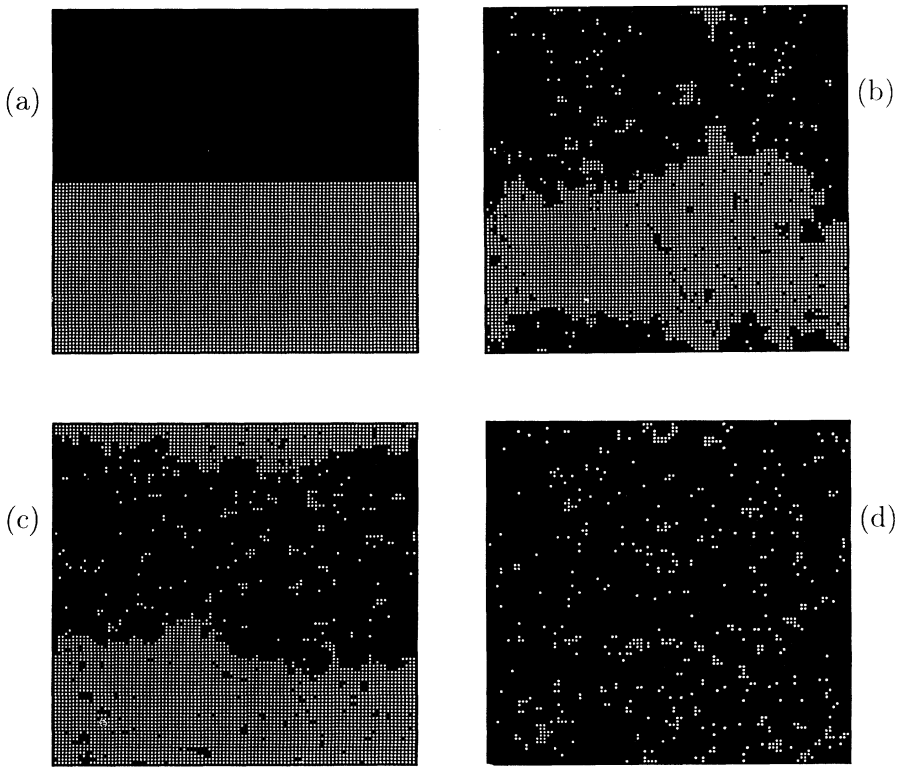

FIG. 3. (a)–(d) Instantaneous spin patterns for the reference system of the dynamical Ising model of Sec. II B. A site with spin $s = +1$ is marked black, a site with $s = -1$ is marked white. (a): $t = 0$; (b): $t = 3000$; (c): $t = 6000$; (d): $t = 9000$. t is the number of time steps. During one time step all sites of the lattice are updated in two full sweeps through the respective black and white checkerboard sublattices of the system.

energy variable is exponentially distributed with weight $P(K_i) \propto \exp(-\beta K_i)$, the temperature $T = 1/\beta$ is defined by the expression for the expectation value of K_i:

$$\langle K_i \rangle = \sum_{\{K_i\}} K_i \exp -\beta K_i \Big/ \sum_{\{K_i\}} \exp -\beta K_i \ .$$

In this equation the sums are over the four values which the kinetic energy K_i may assume and which are listed above. Since only integers are involved, the dynamics of this model is not affected by rounding errors.

For the simulations we put $J = 1$ and use a square lattice with 100×100 sites and periodic boundaries. The initial conditions were chosen such that the upper half of the spins are $+1$ [black in Fig. 3(a)], the lower half -1 [white dots in Fig. 3(a)] making the total magnetization zero. All site kinetic energies were set to zero with the exception of 1500 randomly chosen black sublattice sites of the checkerboard [9] which were assigned a value 12. The temperature of this system, $T = 1.55$, is well below the critical temperature for the magnetic phase transition, $T_c = 2.269$. In Figs. 3(b,c) some intermediate configurations are shown exhibiting quite large fluctuations around zero magnetization before settling—after about 7000 time steps—into a stationary state of almost uniform *positive* magnetization [Fig. 3(d)]. About 89% of the spins are $+1$, and this number fluctuates only slightly. Of course, the notion of a phase transition and of a spontaneous positive magnetization is strictly correct only in the thermodynamic limit of an infinite system [10].

In a second simulation the same initial conditions were used with the exception of two selected next-neighbor lattice sites of the black sublattice (separated only by a single white lattice site in the full checkerboard lattice) the kinetic energies of which, 0 and 12, were interchanged. The initial spin configuration [Fig. 4(a)] is identical to that in Fig. 3(a). The simulation again reveals quite wild fluctuations of the total magnetization around zero [Figs. 4(b,c)] before committing itself—after about 18000 time steps—to a stationary state of almost uniform *negative* magnetization [Fig. 4(d)].

III. MIXING SYSTEMS

For the convenience of the reader we start with a summary of the relevant features of the quantum-mechanical formalism. There the observables are the Hermitian elements of an algebra $\mathcal{A}$. Classically $\mathcal{A}$ is Abelian and consists of the functions $f(q,p)$ on phase space. The time evolution $a \to a_t$, $a \in \mathcal{A}$ is an automorphism of $\mathcal{A}$. Classically this means that f follows the orbits $(q,p) \to (q_t, p_t)$ which are determined by the equations of motion. In quantum field theory $\mathcal{A}$ is the bosonic part of the field algebra which is generated by the local destruction and creation operators α and α^* of particles [canonical commutation relations (CCR) algebra for bosons and canonical anticommutation relations (CAR) algebra for fermions]. A state ω is a normalized positive linear functional which assigns to $a \in \mathcal{A}$ its expectation value $\omega(a)$. Classically ω is given by a probability distribution $w(q,p)$, $\omega(f) = \int dqdpw(q,p)f(q,p)$, and in elementary quantum mechanics it corresponds to a density matrix ρ, $\omega(a) = \mathrm{Tr}\ \rho a$. For the following discussion it is sufficient to consider only the simplest observables,

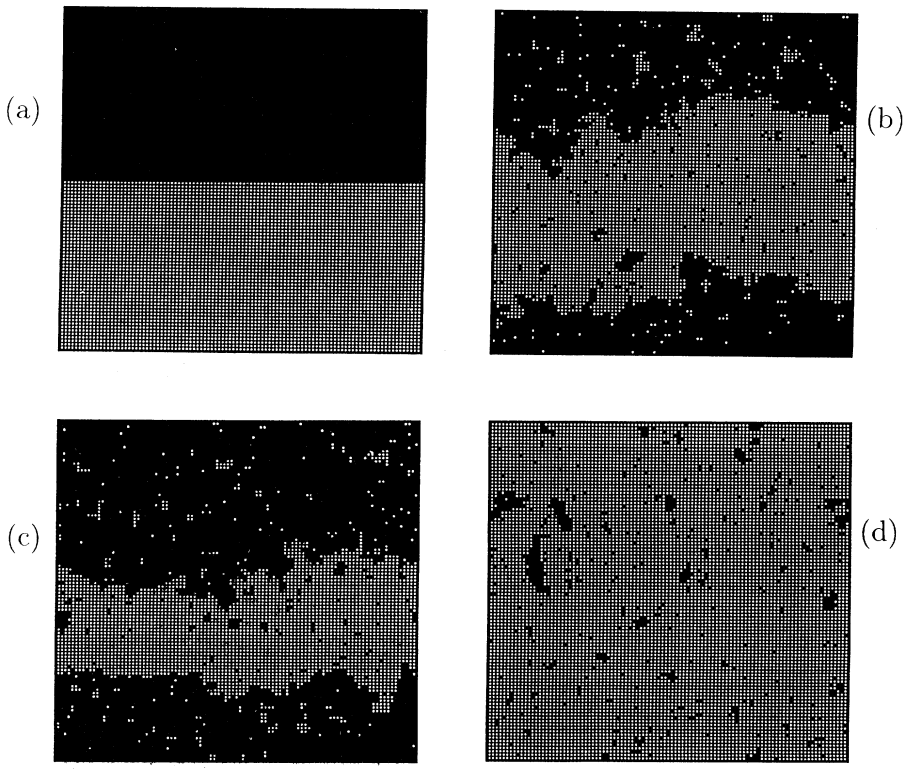

FIG. 4. (a)–(d) Instantaneous spin patterns for the spin system of Sec. II B with slightly modified initial conditions as compared to the reference system of Fig. 3: The kinetic energies, 0 and 12, of two next-neighbor lattice sites of the black checkerboard sublattice were interchanged. (a) $t = 0$; (b) $t = 8000$; (c) $t = 15\,000$; (d) $t = 24\,000$.

namely projections $p = p^2 = p^*$ (propositions). They have only eigenvalues 0 or 1 and are the propositions that certain observables have their values in a particular region F. Thus, classically they are the characteristic function $\chi_F(q,p) = 1$ if $(q,p) \in F \subset \mathbb{R}^{2n}$, 0 otherwise. n is the number of degrees of freedom.

If we have a state with $\omega(p) > 0$, and a measurement of p has the result 1, the state is refined to ω_p,

$$\omega_p(a) = \omega(pap)/\omega(p).$$

For instance, the classical microcanonical state ω is the Liouville measure on the energy shell,

$$\omega(a) = e^{-S} \int \prod_i dq_i dp_i \delta(H(p,q) - E) a(q,p).$$

If we know in addition to the energy E that particle 1 is in a region $F \subset \mathbb{R}^3$, this state is refined to

$$\omega_{\chi_F}(a) = e^{-S} \int \prod_i dq_i dp_i \delta(H(p,q) - E) \chi_F(q_1) a(q,p) \, / \omega(\chi_F),$$

where $\chi_F(q_1) = 1$ for $q_1 \in F$, 0 elsewhere. Furthermore, $\chi_F^2 = \chi_F = \chi_F^*$ has the property of a projection, and $\omega_{\chi_F}(\chi_F) = 1$, so that we are sure that particle 1 is in F. In quantum mechanics, if p is one dimensional $\omega_p(a)$ corresponds to the usual contraction of the wave function, but for quantum field theory in infinite space the local observables do not contain one-dimensional projections since there is always something unobserved outside. Nevertheless, the negation $1 - p$ of a proposition p is also an observable.

The meaning of these notions is illustrated by the following lemma.

Lemma L1. The following statements for propositions are equivalent: (1) $p \Rightarrow q$ ($\Rightarrow$ means logical implication); (2) $p \leq q$ [as operator inequality, which means $\omega(p) \leq \omega(q)\ \forall \omega$]; (3) $pqp = p$; (4) $\forall\ \omega$: $\omega_p(q) = 1$; (5) If $\mathcal{A}$ is Abelian and p (respectively, q) correspond to regions P (respectively, Q) then $P \subset Q$.

Proof. (3) $\Leftrightarrow$ (4) follows from the definition of ω_p; (1) $\Leftrightarrow$ (4): Every observer who has measured $p = 1$ is sure to find $q = 1$; (2) $\Rightarrow$ (3): $q \leq \mathbf{1}$ implies $pqp \leq p$ and $p \leq q$ implies $p \leq pqp$; not (2) $\Rightarrow$ not (3): not (2) implies $\exists \omega$ with $\omega(p) = 1$, $\omega(q) < 1$ but $\omega(p) = 1 \Rightarrow \omega(pqp) = \omega(q)$ and thus $\omega(pqp) < \omega(p)$; (5) $\Leftrightarrow$ (2) is obvious.

For infinite quantum systems a local observation can refine a state ω only to a ω_q, where q is the local observable about which we have gained knowledge. This means roughly that we can measure what we want but not infinitely many things. To discuss the limits on predictability due to the unobserved outside we have to seek properties like (4) of $L1$ which do not depend on ω.

Lemma L2. With the norm $\|a\| = \sup_{\|x\|=1, \|y\|=1} |\langle x|a|y\rangle|$ the following properties of projections p, q are equivalent: (1) $\|pq\| = 1$; (2) $\|qp\| = 1$; (3) $\|pqp\| = 1$; (4) $\|qpq\| = 1$; (5) $\forall \varepsilon > 0\ \exists \omega$ such that $\omega_p(q) > 1 - \varepsilon$; (6) $\forall \varepsilon > 0\ \exists \omega'$ such that $\omega'_q(p) > 1 - \varepsilon$; (7) If $\mathcal{A}$ is Abelian then $P \cap Q \neq \emptyset$.

Proof. (1) $\Leftrightarrow$ (2): follows from $\|a^*\| = \|a\|$; (1) $\Leftrightarrow$ (3) and (2) $\Leftrightarrow$ (4) follow from $\|a^*a\| = \|a\|^2$; (3) $\Leftrightarrow$ (5) and (4) $\Leftrightarrow$ (6) follow since for $a = a^*$ we have $\|a\| = \sup_\omega |\omega(a)|$; (7) $\Leftrightarrow$ (1) The product of the characteristic functions is equal to 1 in $P \cap Q$ and zero otherwise.

How chaotic or unpredictable a quantum system is shall be characterized by the following definition [11–13].

Definition D1. A quantum dynamical system is called mixing if

$$\lim_{t \to +\infty} \|ab_t\| = \|a\| \|b\| \qquad \forall a, b \in \mathcal{A}.$$

An immediate consequence is the following lemma.

Lemma L3. Mixing is equivalent to the following properties: (1) $\lim_{t \to -\infty} \|ab_t\| = \|a\| \|b\|$; (2) $\lim_{t \to \pm\infty} \|b_t a\| = \|a\| \|b\|$; (3) for $a, b > 0$: $\lim_{t \to \pm\infty} \|ab_t a\| = \|a\|^2 \|b\|$.

Proof. Follows from $\|a\| = \|a_t\| = \|a^*\| = \|aa^*\|^{1/2}$.

The concept of mixing merits the following remarks.

(a) Classically mixing means that any region F is so finely distributed over all of phase space that it eventually meets any other region G such that $f_t g \neq 0$.

(b) Mixing systems have to be ergodic, for if there was a constant observable $a = a_t \not\propto \mathbf{1}$ we could take two functions f, g with disjoint support on the spectrum of a such that $0 = f(a)g(a) = f(a)g(a_t) = f(a)g_{-t}(a)$ for all t. Thus, if $\mathcal{A}$ contains a Hamiltonian H with $a_t = e^{iHt} a e^{-iHt}$ the system cannot be mixing.

To make the notion of a mixing system more transparent, we consider two examples which are very similar and with a discrete time.

Example A: The shift of a spin chain. $\forall x \in \mathbb{Z}$ one has spin operators $\vec{\sigma}_x$ which commute on different sites, $[\vec{\sigma}_x, \vec{\sigma}_{x'}] = 0\ \forall x \neq x'$, and $\mathcal{A}$ are the polynomials in the $\vec{\sigma}_x$, that is

$$a \in \mathcal{A} \Leftrightarrow a = \sum_{j \text{ finite}} \prod_i \vec{v}_{i,j} \cdot \vec{\sigma}_{x_i}.$$

The time evolution is just a shift,

$$(\vec{\sigma}_x)_t = \vec{\sigma}_{x+t} \qquad \forall t \in \mathbb{Z}.$$

Since $\|a\bar{a}\| = \|a\| \|\bar{a}\|$ if

$$\bar{a} = \sum_j \prod_i \vec{w}_{i,j} \cdot \vec{\sigma}_{\bar{x}_i} \qquad \text{with } x_i \neq \bar{x}_k\ \forall i, k$$

we see that the system *is mixing*. Actually even the norm closure of $\mathcal{A}$ where the a's are infinite norm convergent sums is also mixing. Evidently a system is mixing if it

has a normdense mixing subsystem.

Example B: The shift on a fermionic chain. $\forall x \in \mathbb{Z}$ one has the fermion operators α_x, α_x^*, $\alpha_x\alpha_{x'}^* + \alpha_{x'}^*\alpha_x = \delta_{xx'}$, and again $(\alpha_x)_t = \alpha_{x+t}$. This system *is not mixing.* Consider the projection $p = (1+e)/2$, $e = \alpha_x + \alpha_x^*$, $e^2 = 1$, and $ee_t + e_te = 0\ \forall t \neq 0$. Thus,

$$pp_tp = \frac{1}{8}[(1+e)(1+e_t)(1+e)]$$
$$= \frac{1}{8}((1+e)^2 + (1-e^2)e_t] = \frac{1+e}{4} = \frac{p}{2}$$

or

$$\|pp_tp\| = \left\|\frac{p}{2}\right\| = \frac{1}{2} \neq \|p\|^3 = 1.$$

Therefore the infinite range of correlations created by anticommutativity destroys the mixing.

It is striking that these two examples have so different mixing properties in spite of their similarity.

The problem of predictability can now be formulated as follows. If we want to be able to predict a property described by a projection q with certainty at time t, we need a measurement p at $t = 0$ such that $\omega(pq_tp)/\omega(p) = 1$, or that the negation $1-q_t$ of q_t is false: $\omega(p(1-q_t)p) = 0$. For a real prediction we also require that this is a property of the dynamics $a \to a_t$ and does not depend on the observer represented by ω. If all observers agree that $1-q_t$ is false this means that $\sup_\omega[\omega(p(1-q_t)p)] = \|p(1-q_t)p\| = 0$. Now it turns out that for the chaotic system we are dealing with there will never be a p such that this holds for all times. This is the content of the following lemma.

Lemma L4. For no proposition q of a mixing system there is a proposition p which for all observers even faintly suggests q for all times in the sense that $\omega_p(q_t) > \varepsilon\ \forall t, \omega$.

Proof. $1-q$ is a proposition $\in \mathcal{A}$ and thus $\forall \varepsilon, p\, \exists\, \omega, T$

$$\omega(p(1-q_t)p) > 1-\varepsilon \qquad \forall t > T.$$

Thus

$$\omega(p) - \omega(pq_tp) > 1-\varepsilon$$

or

$$\omega_p(q_t) < 1 - \frac{1-\varepsilon}{\omega(p)} \leq \varepsilon \qquad \forall t > T.$$

Again some remarks are in order.

(a) Different states correspond to observers with different knowledge. For a mixing system for any two propositions p, q there is a time T such that for all times $t > T$ there is an observer ω which after having measured p considers q_t very likely, $\omega_p(q_t) > 1-\varepsilon$, and another observer $\bar{\omega}$ who considers q_t unlikely, $\bar{\omega}_p(q_t) < \varepsilon$. In this sense the system is indeterministic and undecidable. On the other hand, it is deterministic in the sense that given q and t one can find a proposition $p = q_t$ such that $\omega_p(q_t) = 1$ $\forall \omega$.

(b) For example A given above mixing simply means that no matter how many spins one measures in finite regions there are spins further out which remain undetermined and thus there are some initial states which predict them to be up and others which predict them down. On the other hand, in the nonmixing example B once one has measured p any observer predicts a 50% chance of finding $p_t = 1\ \forall\ t \neq 0$.

We have thus shown that mixing systems possess some unpredictability. The question remains as to what physical systems are known to be mixing. In this respect we have the following results [14]:

Theorem T1. For certain smoothed-out Galilei invariant two-body interactions the time evolution is an automorphism of the CAR algebra. There the observables are a mixing system.

Conjecture C1. The observables of Poincaré invariant quantum field theories are a mixing system.

Remarks. C1 is still on the level of a conjecture because in $3+1$ dimensions except for free fields it has not been shown that the time evolution exists as an automorphism of the CCR and CAR algebras. However, the proof of the theorem $T1$ suggests that from the point of view of mixing the Poincaré group is easily as good as the Galilei group. Therefore one expects the theory of everything also to be mixing and to contain the same unpredictability.

IV. CONCLUDING REMARKS

In the simple classical models of Sec. II the different symmetry breakings were all equivalent and therefore do not illustrate the emergence of different laws of nature. Non-equivalent symmetry breakings will reduce a larger group to nonconjugate subgroups. For example, in crystallizing carbon a diamond or graphite structure may emerge. The latter is energetically favored and more abundant. Thus, the question remains why in a theory with a large symmetry group, say some $U(n)$, $n \sim 10$, a breaking into a particular subgroup, say some $U(n_1) \times U(n_2)$, $n_1 + n_2 \leq n$, should be favored.

Our result does not mean that the theory does not contain some statements which can be made with certainty. For instance, in the spin chain of Sec. II one can state with certainty that the spin at each site is $\frac{1}{2}$, since $\left(\frac{\vec{\sigma}_i}{2}\right)^2 = \frac{1}{2}\left(\frac{1}{2}+1\right)$. This means that the observable is a multiple of unity and $\omega(\vec{\sigma}_i^2) = 3\ \forall i, \omega$. In some representation the average magnetization $\vec{m} = \lim_{N\to\infty} \frac{1}{2N+1}\sum_{i=-N}^{N} \vec{\sigma}_i$ may exist and is translation invariant. If it is not represented by a multiple of unity the system is not mixing. This does not contradict our statement in Sec. III since this is not a local observable but presupposes some global knowledge.

The situation in mixing systems has some similarity to what happens in formal mathematical systems. As Gödel has shown the latter also contain undecidable propositions in the sense that neither they nor their negation can be proved. The element which appears in the discussion of mixing systems is the uniformity in time.

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