Classical and quantum irreversibility

B B Kadomtsev

Contents

Abstract. Irreversibility of physical systems is discussed by considering the simplest example of a low-density gas, either in isolation or in thermal equilbrium with the walls of a container. Attention is concentrated on an analysis of a logical scheme for a theoretical description of irreversibility.

1. Introduction

Irreversibility is a universal principle of the Universe, which applies not only to life, but also to many physical phenomena in nature. It would not be an exaggeration to say that we are immersed in an irreversible gradually evolving Universe. However, the classical laws of mechanics are reversible in time. The main equations of quantum mechanics are also reversible. Therefore, the question of how a description of irreversible processes can be derived from the reversible equations of dynamics has been discussed repeatedly and continues to be discussed in the physics literature. I do not wish to comment here on all the points of view on this topic. I shall set myself a simpler task: I shall take as an example one of the simplest physical systems with an inherent internal irreversibility and I shall try to analyse more carefully the logical reasoning scheme resulting in a theoretical description of irreversibility. I shall select a low-density gas of weakly interacting atoms as the simplest system. I shall assume that the gas is inside a closed container and it may be in thermal equilibrium, including equilibrium with uniformly heated container walls.

It is known that the behaviour of such a gas is described by the Boltzmann kinetic (transport) equation for the particle distribution function $F(r, v, t)$, where r is the coordinate (a three-dimensional vector) and v is the velocity of a particle. All the particles are assumed to be characterised by the same distribution function, so that $F = nf(r, v, t)$, where n is the particle density and $f(r, v, t)$ is the single-particle distribution function.

Boltzmann deduced his kinetic equation with the help of just one perfectly natural assumption: the atoms in a gas are assumed to be uncorrelated before their pair collisions. Boltzmann called this the 'molecular chaos' hypothesis. This hypothesis seems quite natural, although in no way does it follow from molecular dynamics.

It has been proved that just this hypothesis is quite sufficient to introduce physical irreversibility explicitly: according to the famous H theorem, the kinetic equation describes irreversible relaxation of a gas to thermodynamic equilibrium accompanied by a monotonic increase of the entropy with time. The question arises as to which physical phenomenon underlies the hypothesis of molecular chaos and how this phenomenon can be considered within the framework of a more rigorous logical scheme. This is the question which will be discussed here. I shall begin with a gas of classical particles and discuss later a more rigorous quantum description of the behaviour of atoms.

2. Classical irreversibility

In the approximation of classical particles we can regard the atoms as tiny hard balls colliding elastically with one another. If the diameter of these balls is d, the collisions occur for impact parameters smaller than d. This means that the scattering cross section is $\sigma = \pi d^2$ and the mean free path is $\lambda = 1/n\sigma$, where n is the average density of atoms. The gas is considered to be of low density if $\lambda \gg \sqrt{\sigma}$, i.e. if $n\sigma^{3/2} \ll 1$.

We shall assume first that the gas is inside a container of volume V with ideally (specularly) reflecting walls. The total number of atoms in the volume V, equal to $N = nV$, will be regarded as very large: $N \gg 1$. We can easily see that such a system of elastically interacting particles is fully reversible in time. In fact, the potential of the interaction of the particles

B B Kadomtsev Institute of Nuclear Fusion, Russian Scientific Centre 'Kurchatov Institute', pl. Kurchatova 46, 123182 Moscow
Tel. (095) 196 98 14. Fax (095) 190 42 44.
E-mail: kadomtsev@ufn.msk.su

with one another and with the container walls depends only on the coordinates. Therefore, Newton's equations are not affected by the replacement of t with $-t$. This means that for any initial state $t = 0$ a system of classical elastic particles evolves up to a moment t reaching such a state that after time reversal the system exactly repeats its evolution in the reverse order. Naturally, such a 'reverse cinema' scenario can be realised also by instantaneous transformation of the velocities $v_i \rightarrow -v_i$ for each ith particle from the total set of N particles. Thus, molecular mechanics of a gas is reversible in time, which is clearly in conflict with the reality that we experience.
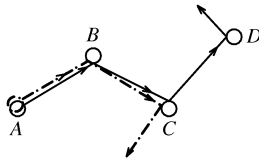
Figure 1. As a result of a small displacement of an atom A, its path (dotted line) begins to deviate significantly from its initial path (continuous line) after the very first few collisions with other atoms.

We can understand the origin of irreversibility by considering in greater detail the dynamics of gas atoms. Let us select a test particle A (Fig. 1). Such a particle travels freely for a time. Its velocity then changes instantaneously because of a collision with another atom B, and it flies on to the next collision. The average length of such free–flight segments is λ, i.e. it is equal to the mean free path. The average time between consecutive collisions is $\tau = \lambda/v_t$, where v_t is the average velocity of a particle. The path of a specific test particle is very sensitive to the specific positions and partners in pair collisions with the other particles. Therefore, such a path is random and the corresponding process is known as dynamic chaos. In our case, dynamic chaos is related to the large number of partners that participate in collisions. However, it is well known that dynamic chaos occurs also in systems with few degrees of freedom.

Dynamic chaos by itself cannot account for the appearance of irreversibility. No matter how complex is the evolution of a system from the past to the future, a closed system of classical particles must follow in the reverse order the same path in the phase space when t is replaced with $-t$. Therefore, irreversibility is not a direct consequence of chaos although it may be related indirectly to chaos.

To proceed further, we must consider one other feature of chaotic systems which is the divergence of the paths in the phase space. Once again, let us consider a test particle (Fig. 1) and examine not only its real path, but a possible path lying close to it. For example, we can assume that the test particle is displaced slightly by a very small distance ξ. Then, after the first collision the scattering direction changes by a small angle $\gamma_0 \cong \xi/a$, where $a = \sqrt{\sigma}$ is a characteristic interaction length. A small deviation γ alters the impact parameter by $\gamma\lambda$ in the second collision, so that after the second scattering the direction of motion of the test particles changes by $\gamma_1 \sim (\xi/a)\cdot(\lambda/a)$. After q scattering events, the angle becomes approximately $\gamma_q = (\xi/a)\cdot(\lambda/a)^q$. Since $\lambda/a \gg 1$, the value of the angle γ_q increases rapidly

with the number of scattering events. If $\gamma_q \sim 1$, the particle path jumps to the next atom and the perturbed particle path becomes quite different from the initial one. For example, after $q \cong \ln(a/\xi)/\ln(\lambda/a)$ scattering events a particle follows a very different path. In other words, the initially close paths begin to diverge exponentially. This divergence of the paths results eventually in irreversibility. However, we must also understand how this occurs.

As shown above, there is no irreversibility in a closed system of classical particles. However, even negligible external perturbations are sufficient for the appearance of irreversibility. We can see that it is sufficient to displace one of the colliding atoms by just $\xi \sim a^2/\lambda = \sigma/\lambda$ to ensure that after one or two collisions the particle paths become completely different from the initial paths when $\xi = 0$. The quantity $\xi \sim \sigma/\lambda$ is negligible; for example, in atmospheric air at normal pressure we have $\xi \sim 10^{-7} \lambda \sim 10^{-11}$ cm. If we assume that the gas is in a larger or smaller container i.e. if we take account of the feasibility of heat exchange with the walls because of inelastic collisions, then displacements on this scale are quite likely even far from the walls. Near a wall the elastic collisions of atoms with it may result in displacements of the order of λ and then perturbations are transferred into the gas interior either by diffusion or by acoustic noise, which is generated near the walls because of inelastic collisions. Such collisions contribute to the additional attenuation of acoustic waves and, according to the fluctuation–dissipation theorem, the wall layers of a gas can generate additional acoustic noise. This noise may result in displacements of atoms within the gas and thus transfer atoms from some unstable paths to others.

It is these external perturbations that create irreversibility. They can be regarded as a certain type of chaotic noise. Therefore, molecular dynamics can be considered as a special 'chaos amplifier' with respect to the arrival of external noise. The 'amplifier' has an enormous gain. The number of collisions needed to displace paths depends only logarithmically on the external noise intensity. Therefore, even a very weak interaction with the environment radically alters the behaviour of the gas atoms. All the long-range correlations of atoms are destroyed very rapidly: this happens over a period of just one or two typical pair collision times. The behaviour of atoms with the same initial velocities thus becomes monotypic: they move and collide with other atoms in accordance with the same statistical laws. Consequently, a many-particle distribution function is transformed into a product of single-particle distribution functions which obey the Boltzmann equation.

It follows that, strictly speaking, molecular chaos in a gas of classical particles is created by the external environment. Clearly the behaviour of such a gas becomes irreversible: we could reverse the velocities of molecules inside the container, but the external environment is outside our control. Therefore, reversibility for $t \rightarrow -t$ can exist for a period not greater than one or two mean collision times and then the gas again forgets its initial state and its evolution is exactly the same as at $t > 0$ (but with the reversed gas dynamic velocities).

We can therefore see that irreversibility can appear without energy transfer to or removal from a gas. Paths become chaotic simply because of small displacements of atoms, i.e. due to a characteristic 'dephasing' in the pair collision processes. Irreversibility is unrelated to energy changes.

We can understand better the nature of classical irreversibility by considering an idealised thought experiment. Let us consider a gas with the density of atoms n in a spherical container of radius R with specularly reflecting walls. Such a gas is clearly an ideal mechanical system with motion fully reversible in time. Let us now assume that the container walls are very thin and that outside the container there is exactly the same gas with the same average velocity of thermal motion of atoms and with the same density n. Let both gases be on the average at rest. Let us assume that the external gas is in a state of thermal equilibrium and that its interaction with the external Universe is such that molecular chaos is established inside the gas. We shall assume that the mean free path λ is much less than the container radius R.

Let us assume that at the moment $t = 0$ the wall separating the two gases disappears. An initial discontinuity then separates the two gases: the external gas which is in thermal equilibrium and the internal system of atoms which is in complex but fully reversible motion. Clearly, the random thermal motion of the external gas together with the acoustic thermal noise should lead to chaotisation of the paths of the atoms of the internal gas. One collision of the chaotised gas is sufficient for dephasing of the path of an internal-gas atom. An irreversible front therefore begins to propagate inside the region with reversible motion of atoms (Fig. 2). Ahead of this front the motion is still reversible, but behind, it is irreversible. In other words, a reversibility-destroying front propagates inside the gas.
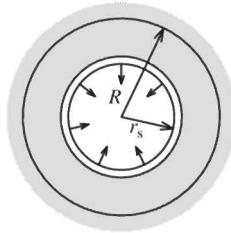
Figure 2. Irreversibility front of radius r_s collapses towards the centre at the velocity of sound after the disappearance of a shell of radius R separating an internal reversible gas from an external irreversible environment.

It is known that any travelling weak discontinuity in a gas propagates at the velocity of sound, $c_s = (\gamma T/m)^{1/2}$, where γ is the adiabatic exponent, T is the absolute temperature, and m is the mass of an atom. The radius of a sphere r_s with reversible motion inside it will correspondingly contract in accordance with the law $r_s = R - c_s t$. At $t = R/c_s$ the reversible region disappears. An equilibrium gas with the usual random paths of atoms and with destroyed long-range correlations between their motions forms behind the moving front. The correlations in the motions of atoms are destroyed in the front itself, the width of which is of the order of λ. Ahead of the front we have a classical mechanical system with a perfectly determinate and, therefore, unique path in the phase front. The replacement of t with $-t$ in this system simply reverses the direction of motion of the system along a path. We should therefore assume that there is no disordered motion inside the sphere of radius r_s. This means that the entropy of the

system of atoms inside the sphere of radius r_s is zero. Immediately after the passage of the front this equilibrium gas acquires an entropy S (per unit volume), which can be calculated in accordance with the familiar methods of statistical physics.

The main physical process occurring at the moving front thus involves entropy creation beginning from zero to the value S per unit volume. The process of entropy creation is irreversible and, therefore, the irreversibility front can move only in one direction: towards the reversible mechanical system of particles with zero entropy.

We shall now have to consider how and from what entropy is created. We shall do this by applying the well-known Boltzmann formula:

$$S = k \ln \Gamma. \tag{1}$$

Here, Γ is the number of possible microscopic states of a system when its macroscopic parameters (for example, the gas density and temperature) are fixed. The parameter k, known as the Boltzmann constant, appears because the absolute temperature is measured in kelvins and the energy of an atom is measured in ergs or joules. If we agree to measure the absolute temperature in the same energy units as the energy of atoms, we can assume that $k = 1$. This choice of units is more convenient, so that we shall postulate that $k = 1$ in formula (1).

In classical mechanics the numbers of states Γ is not defined rigorously. However, if following the uncertainty principle $\Delta x \Delta p \approx \hbar$, we divide the whole phase space into discrete cells of size Δx and Δp, so that $\Delta x \Delta p \approx \hbar$, the value of Γ becomes fully determinate.

We shall agree to use the same discrete cellular space to describe the mechanical motion of a system of classical particles also. We then encounter immediately the concept of information. Let us consider our mechanical system of atoms at some fixed moment in time. At this moment the phase point of this system is a unique one cell out of Γ possible cells. We can see that the probability of finding the system in this cell is $p = 1/\Gamma$. If all the possible cells are taken into account, the system of atoms can be regarded as a memory with the information capacity

$$I = -\ln p = \ln \Gamma. \tag{2}$$

This is exactly the information carried by a classical system of atoms at any moment in time. During evolution in time the phase point moves along a very narrow (of width amounting to one cell) filament in the phase space, so that its information is conserved.

In the Shannon relationship (2), information is measured in 'nats' and not in bits, so that the link between this relationship and the entropy given by formula (1) with $k = 1$ becomes obvious. If information is erased completely, the system of atoms can be in any one of the possible cells, the number of which is Γ. Perfectly random thermal motion is then established.

Thus, complete erasure of information and its conversion into entropy occurs at the irreversibility front. Ahead of the front we have a mechanical system with a fully determinate behaviour in time, but behind the front we have thermal motion chaos. We must stress once again that this chaos is created by an infinitesimally weak noise from the irreversible external environment. The dynamics of atoms in the gas amplifies this chaos by a large factor and converts it into the molecular chaos of thermal motion.

We shall now consider some problems encountered in various textbooks on thermodynamics and statistical physics or simply in popular papers on physics. For example, one of the frequently asked questions is as follows: is there an instantaneous temperature? Paradoxically, for a gas of classical particles the answer should be negative: there is no instantaneous temperature.

In fact, any instantaneous state of a system of classical particles should be regarded as specified exactly, i.e. as having zero entropy and total information $I = \ln \Gamma$. Therefore, we cannot introduce the instantaneous temperature concept (we can assume that this temperature is zero, but this is not very significant). Only in the presence of weak external perturbations, amplified by the pair collisions of particles after a time interval of the order of the mean collision time, do we encounter real molecular chaos with the corresponding temperature which is a measure of the chaotic thermal motion. Any initial information then disappears and the entropy reaches its maximum value $S = \ln \Gamma$. It is this process of the appearance of temperature with simultaneous conversion of information into entropy which occurs in the narrow layer of an irreversibility front shown in Fig. 2.

The second frequently asked question is: why is it possible to use a statistical approach to the description of the behaviour of a gas of classical particles? Various answers have been given. It is sometimes said that a statistical description is used because the exact initial data are not known. One can also encounter the statement that statistics is used because it is not possible to integrate the equations of motion for an enormous number of particles. It is easy to see that neither of these two answers can be regarded as fully correct.

We shall begin with the second answer. In normal air under atmospheric pressure in a volume of the order of λ^3 there are $N = 1/\sigma^3 n^2 \sim 10^8$ particles. This is of course a large, but not an enormous number. The entropy $S = \ln \Gamma$ of N gas molecules at room temperature is approximately $S \cong N \times 30 = 3 \times 10^9$. Consequently, the information carried by the initial state is measured in gigabytes, which can be dealt with quite readily by a modern computer. A supercomputer can carry out calculations analysing the evolution of gas molecules for a certain number of pair collisions. If desirable or essential, it is possible to simulate gas dynamics in the approximation of enlarged particles.

Let us now consider the first answer. Strictly speaking, the fact that we do not know the initial data does not give us any right to employ a probabilistic description. After all, such a description should be applied not to many repeated measurements but to one natural system. This system is closed and evolves along a single path in the phase space. The replacement of such a system with an ensemble of systems with somewhat different initial data is not only logically unjustified, but leads to certain logical difficulties.

In fact, the uncertainty about the initial data can be allowed for by the creation at $t = 0$ of a 'drop' of the distribution function in the phase space. During the subsequent evolution of a closed system each point of such a drop moves along a unique rigorously defined path. The paths diverge, so that very soon a 'cotton wool' or 'spider's web' is formed and it is filled with points of the initial distribution function. It is usual to carry out 'coarse-grained averaging' in order to simplify the description of this cotton wool. However, this averaging operation is not justified in any way: it is artificial and imposed from outside. Only a real disturbance of the paths by an external noise creates conditions justifying such averaging.

We thus can draw once again the conclusion that irreversibility of a gas of classical particles and the justification for its statistical description are determined by a very weak interaction of the investigated system with an irreversible external environment. Collisions of particles greatly amplify the external chaotic perturbations and destroy the long-range correlations in the motion of particles. As a result, this motion becomes monotypic: every particle behaves similarly and can be characterised by a single-particle probabilistic distribution function. The Boltzmann equation is formulated precisely for this function.

The macroscopic characteristics of a gas can behave similarly in a closed system and in a system which is in contact with the external world. However, the hypothesis of molecular chaos is logically justified only if we assume that the gas in question is characterised by a very weak interaction with the irreversible external world. Closed and open systems differ greatly from the logical point of view.

3. Quantum irreversibility

Quantum irreversibility differs greatly from classical irreversibility, but the reasoning used in the preceding section can help here as well.

Let us again assume that we are dealing with a closed system of atoms in a container with specularly reflecting walls. We shall assume that the gas temperature is considerably higher than the degeneracy temperature, so that the behaviour of atoms can be near-classical. We can readily see that in a closed system we again have full reversibility. In fact, the behaviour of this system is described by the Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi . \tag{3}$$

Here, $\hbar$ is the Planck constant, H is the Hamiltonian, and ψ is the wave function which is symmetric in N variables $r_1 \ldots r_N$.

It follows from Eqn (3) that the wave function $\psi(r, t)$, where r is the set of variables r_i, can be found from its initial value $\psi(r, 0)$ by the operation

$$\psi(r, t) = \exp\left(-\frac{iHt}{\hbar}\right)\psi(r, 0) . \tag{4}$$

The matrix $U(t) = \exp(-iHt/\hbar)$ is unitary, so that $U^{-1}(t) = \exp(iHt/\hbar)$. We have therefore the corresponding relationship

$$\psi(r, 0) = U^{-1}(t)\psi(r, t) = \exp\left(\frac{iHt}{\hbar}\right)\psi(r, t). \tag{5}$$

In other words, the function $\psi(r, 0)$ can be found from a given function $\psi(r, t)$ by means of relationship (4) but with reversed time: $t \rightarrow -t$. It therefore follows that relationships (4) and (5) correspond to the statement that a closed quantum system is fully reversible.

Consequently, the irreversibility can appear only as a result of a weak interaction of the investigated system with an irreversible external environment.

It is convenient to begin by considering a certain thought experiment in a closed system in order to understand how the irreversibility appears in a gas of

quantum particles. Let us assume that at some initial moment $t = 0$ the wave function of N particles has the general form $\psi(r, 0)$, where r is a set of N coordinates of the r_i type. We shall select a test particle, for example, one with the coordinate r_1. We shall avoid complications associated with the identity of the particles by postulating that the test particle (atom) has an isomeric nucleus, i.e. there is no complete identity between this atom and others, although the masses of all the atoms are the same. We shall now represent the function $\psi(r, 0)$ by a super-position

$$\psi(r, 0) = \sum_j \psi_j(r_1) C_j. \qquad (6)$$

Here, each of the functions $\psi_j(r_1)$ is selected in the form of a wave packet labelled by a certain number j and the coefficients C_j represent the wave functions of all the remaining atoms in the selected state with the wave function $\psi_j(r_1)$ of the first atom.

Let us select the width Λ of a wave packet $\psi_j(r_1)$ in such a way that this packet does not broaden very significantly in the time $\tau = \lambda/v_t$, where λ is the mean free path and v_t is the average 'thermal' velocity of the atoms. It follows from the uncertainty principle,

$$\Delta p \Delta x \approx \hbar, \qquad (7)$$

that the velocity uncertainty in a packet of width $\Delta x \sim \Lambda$ is $\Delta v \sim \hbar/m\Lambda$, where m is the mass of an atom. Our condition $\tau \cdot \Delta v \approx \Lambda$ thus leads to the approximate relationship:

$$\Lambda^2 \cong \lambda \lambda_B, \qquad (8)$$

where λ_B is the de Broglie wavelength: $\lambda_B = \hbar/m v_t$.

We shall now consider the evolution of the wave packet $\psi_j(r_1, t)$ with time. In a low-density gas this packet travels freely most of the time and is scattered weakly by other atoms. In the time $\tau = \lambda/v_t$ the initial packet is almost completely converted into scattered waves. These waves undergo secondary scattering and then tertiary scattering, and so on. Let us now 'reverse the time' again, i.e. let us replace t with $-t$. Then all the scattered diverging waves transform into converging waves and the whole wave evolution occurs in the reverse order, until these waves coalesce into the initial wave packet $\psi_j(r_1, 0)$. Hence, it follows that in a reversible system of quantum particles we should encounter in equal measure both diverging (scattered) waves and converging waves. The wave function of such a system is a very complex and fine construct of perfectly correlated converging and diverging waves.

Let us now assume that the gas under investigation interacts weakly with an irreversible external environment. The first and main effect of this interaction is to destroy the exact phase relationships between the converging and diverging waves. This is called dephasing. Clearly, such dephasing has an influence primarily on the disappearance of the converging waves, similar to the emission waves in ordinary classical electrodynamics.

The converging waves can be excluded mathematically by postulating weak attenuation of the scattered waves at large distances from the scattering point. An approach of this kind is employed in quantum mechanics when the optical model of a nucleus is considered: a nucleus is regarded simply as a ball of gray matter when a neutron is scattered. The hypothesis underlying this approach is that the wave function of a neutron which becomes 'entangled'
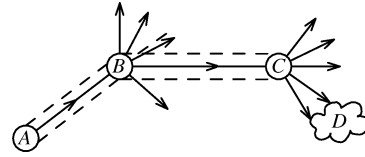
Figure 3. Wave packet A is scattered by another atom in region B and then one of the scattered waves is scattered in region C by a third atom. It is assumed that a single 'extended collapse' occurs in region D. Then, returning back in time to point A, we can reproduce the motion of the wave packet and its subsequent collisions.

in the nucleus cannot be superimposed on the incoming wave function of a free neutron.

For a gas of quantum particles it is also natural to assume that the initial wave function $\psi_j(r_1)$ gradually disappears over a distance $\sim \lambda$ and is converted into scattered waves. However, this is insufficient. A quantum particle cannot become manifest simultaneously in many parts of space under conditions such that the coherence between these parts is destroyed completely. It is therefore essential to adopt as an axiom the statement that, after a certain time interval, which is of the order of several scattering times, the wave function of a particle can differ from zero only in a certain limited region of space. This region is identified by a letter D in Fig. 3. The effect which occurs can be called the wave function 'collapse'. However, it should be stressed that we are dealing mainly here not with 'contraction' of the wave function into region D, but with 'annihilation' of the wave function outside a certain wide region D.

In the course of the 'collapse process' the wave function of a particle is distorted and it would seem that it is distorted very strongly: after all, it is destroyed over a large part of space. However, the dynamic perturbation of the system can still be very small. The wave function is after all constructed in such a way that not the function itself but the operators with weight $|\psi|^2$ are the physical quantities. Consequently, a wave function should be regarded as information rather than as a dynamic quantity. Therefore, introduction into a wave function of a localisation form factor which is extended in space may not greatly influence the dynamic properties (for example, energy). However, it can very strongly affect the information characteristics of the wave field.

We shall therefore assume that the influence of an external environment results in the disappearance of converging waves and leads to a situation in which a wave packet of a test particle contracts sooner or later in a certain region D in Fig. 3. We can now use the inverse transformation in time to return to the initial region A. Since we are left with just the scattered waves, it follows that in region C of the preceding collision the wave function is already compressed into a packet of size of the order of Λ and this packet can be traced as it moves from point C to B and from point B to A. It follows from the Einstein–Podolsky–Rosen paradox [1] that a similar collapse occurs also in the wave functions of the atoms on which the scattering takes place. We can say that any extended collapse in future is equivalent to the fact that at present the evolution of the wave function $\psi_j(r_1)$ can be regarded as the result of free motion of the packet along rectilinear segments with random collisions in regions B, C, etc. A

quantum particle not only reveals features of classical behaviour, but its behaviour is random in each scattering event.

A statistical description of such quantum objects can be provided in a natural manner by introducing the density matrix for an ensemble of identical systems, i.e. initially for similarly behaving atoms. The diagonal terms of the single-particle density matrix, i.e. $|\psi_j(r_1)|^2$, then play the role of the distribution function and the 'erasure' of the off-diagonal terms corresponds to the process of formation of a packet. In this approach all the atoms behave in the same way and any 'instantaneous' wave function $\psi(r, t)$ of many atoms can be regarded as a random set of wave packets whose probabilistic characteristics are described by the kinetic equation for the distribution function and by an additional equation for the shape and dimensions of the wave packets.

We can therefore draw the conclusion that even a weak effect of an irreversible environment can greatly alter the wave function of a system of quantum particles. Instead of a complex coherent state with evolution reversible in time, we have a set of single-particle wave packets with random irreversible evolution. The irreversibility appears over time intervals longer than the mean collision time and the actual difference between the wave functions of closed and open systems can have a much more complex space–time structure.

This question can be understood better by returning to Fig. 2, but for the case of a gas of quantum particles. As in the classical case, the encounter between a pure state and an irreversible external environment creates an irreversibility front which collapses at the velocity of sound. A reversible pure state organised in a complex manner exists ahead of this irreversibility front. Behind the front a set of random single-particle wave packets is formed. Such a state can naturally be called mixed, because the behaviour of each of the packets is random and it obeys probabilistic laws. It is natural to assume that the width of the irreversibility front is characteristically of the order of the mean free path λ, although in general the situation may be somewhat complex because more distant interatomic quantum correlations may be destroyed ahead of the irreversibility front. The localisation (collapse) of the wave function of any atom corresponds to a 'measurement' of its coordinate and, therefore, the wave function of a gas of the remaining atoms can react instantaneously to such a measurement by annihiliation of some of its components.

We can thus see that the wave functions of closed and open systems are different. The wave function of an open system behaves as a set of a large number of wave packets. Such a set of packets cannot be regarded as a pure state of the general type. Therefore, in the case of a quantum system (in contrast to a classical system), we are fully justified in speaking of an instantaneous temperature: the wave function of a system in thermal equilibium is known to differ strongly from any pure state. At any moment this function can be regarded as a set of wave packets with Maxwellian distribution of the momenta.

It is not possible to identify the exact moment of collapse of the scattered waves. We, therefore, may assume that the collapse represents a process extended in time without fixed intermediate states. This approach differs from the usual quantum mechanics formulated solely for reversible systems.

4. Schrodinger's cat paradox

An example of a characteristic quantum irreversibility is Schrodinger's famous thought experiment [2]. It is known as the 'Schrodinger's cat paradox'. It is assumed in this paradox that a Geiger counter, recording α particles crossing it and originating from decay of radioactive nuclei, is brought into contact with a device which is used to break an ampoule containing potassium cyanide when a particle is recorded. This device and a live cat are placed under a glass dome. According to standard quantum mechanics, we can image a superposition of two states of the counter in which the flight of an α particle is recorded or unrecorded. However, this results in a superposition of a live cat with a dead one.

It is understood that without an α particle nobody could think up such a strong superposition. The crux of the matter is in a microparticle, which by definition should be described by quantum mechanics. This particle interacts with a more complex system, which is a Geiger counter, and via this counter with an ampoule and then finally with a cat. A natural approach to the description of the whole process is to extend the system from the α particle to the counter, etc. This involves a gradual increase in the number of the dynamic variables and widens the Hilbertian space where the wave function is defined. It seems that at each step one should use the Schrodinger equation. The result is the possibility of an absurd superposition of two irreversible processes.

It is clear that the main conclusion from this discussion is that the reversible Schrodinger equation is unsuitable for the description of irreversible processes (it should be noted, however, that this is not generally accepted). We have seen above that a very weak interaction with an irreversible external environment greatly influences the irreversible evolution of a complex quantum system. Therefore, the description of such a system differs from a simple application of the Schrodinger equation.

In the case under discussion the Schrodinger equation describes α decay of a nucleus and a spherically symmetric wave function of an escaping α particle. If the radioactive nucleus is in air, the Schrodinger equation for the extended system describes the scattering of gas atoms by the α particle and possible ionisation of these atoms. However, reversible evolution of this system lasts only for a time of the order of the free flight time of the gas atoms. This is followed by the collapse of the wave packets of the gas atoms, accompanied by the collapse of the wave function of the α particle: from spherically symmetric, this wave function is converted into a freely travelling localised packet accompanied by a wake of scattered and ionised atoms. This evidently irreversible process can be regarded as a transition of a system from one Hilbertian space to another, accompanied by complete disappearance of the initial spherically symmetric wave function. If vacuum separates the radioactive nucleus from the Geiger counter, then the collapse process occurs in the counter itself. It is this process that finally results in the unavoidable sad fate of the cat.

It thus follows that there can be no superposition of the live and dead cats in a logically justified approach to the description of irreversible processes: a process can follow only one of several possible irreversible scenarios. One must not apply literally the reversible form of the Schrodinger

equation and one should introduce the collapse of wave functions into the scenario of their evolution.

5. Conclusions

The irreversibility of the processes that occur in physical systems, which may be classical or quantum, is continuing to be the subject of discussion and various points of view are being put forward even now. The question of irreversibility at the interface between classical and quantum systems is particularly topical, especially when measurements of quantum systems are considered. There is no generally accepted theory of quantum measurements and the main difficulty encountered in developing it is the theory of irreversible phenomena.

A low-density gas at a moderately low temperature is a convenient object for discussing the irreversibility problems. The irreversibility of a classical gas has been considered from many points of view, beginning from the outstanding work of Boltzmann. The irreversibility in a quantum gas has been also the subject of fairly profound theoretical analyses. The need to consider the irreversibility at the microscopic level, i.e. in quantum processes, has been stressed repeatedly by Prigogine and his colleagues [3 – 5]. They have drawn special attention to the fact that the classical limit of a low-density gas corresponds to classical chaos with diverging paths in the phase space without integrals of motion. Therefore, Prigogine and his colleagues have tried to develop such a mathematical approach for the description of this situation which would lead automatically to the collapse of wave functions.

The problem of irreversibility at the level of a clear description by means of thought experiments is discussed above. The stress is on a logical way of developing the relevant considerations. These considerations unavoidably lead to the conclusion that the origin of irreversibility lies outside a system of many atoms under discussion. It is shown that a low-density gas is a very effective amplifier of external noise. In a gas of classical particles such 'chaos amplification' appears because of instability of the paths of the atoms. In the quantum case the influence of the external environment in the form of a 'collapse seed' in the future leads to decay of the wave function into a set of wave packets resembling 'extended' classical particles. The interaction of such packets with one another appears as a random process of pair collisions, which can be described by the kinetic equation for the single-particle distribution function. It is to be hoped that a more rigorous quantum theory of irreversible processes will be developed.

References

1. Einstein A, Podolsky B, Rosen N *Phys. Rev.* **47** 777 (1935)
2. Schrodinger E *Naturwissenschaften* **23** 807, 844 (1935)
3. Prigogine I *From Being to Becoming: Time and Complexity in Physical Sciences* (San Francisco: W H Freeman, 1980)
4. Prigogine I, Stengers I *Order Out of Chaos: Man's New Dialogue with Nature* (New York: Bantam Books, 1984)
5. Petrosky T, Prigogine I *Phys. Lett. A* **182** 5 (1993)