Is thermodynamic irreversibility a consequence of the expansion of the Universe?

Szabolcs Osváth

szabolcs.osvath@gmail.com

Department of Biophysics and Radiation Biology

Semmelweis University, Tűzoltó u. 37, Budapest

H-1094, Hungary

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This paper explains thermodynamic irreversibility by applying the expansion of the Universe to thermodynamic systems. The effect of metric expansion is immeasurably small on shorter scales than intergalactic distances. Multi-particle systems, however, are chaotic, and amplify any small disturbance exponentially. Metric expansion gives rise to time-asymmetric behavior in thermodynamic systems in a short time (few nanoseconds in air, few ten picoseconds in water). In contrast to existing publications, this paper explains without any additional assumptions the rise of thermodynamic irreversibility from the underlying reversible mechanics of particles. Calculations for the special case which assumes FLRW metric, slow motions ($v \ll c$) and approximates space locally by Euclidean space show that metric expansion causes entropy increase in isolated systems. The rise of time-asymmetry, however, is not affected by these assumptions. Any influence of the expansion of the Universe on the local metric causes a coupling between local mechanics and evolution of the Universe.

1. Introduction

Many examples of statistical mechanics show how classical mechanics can grab the essence of phenomena using the particle model of matter. In the Hamiltonian formulation of classical mechanics, a system of N particles is described by 3N coordinates and 3N momenta, which are usually combined in a 6N dimensional phase space. Every possible state of the system is represented as a point in the phase space in which the time evolution of the system plots a trajectory. The time dependence of the coordinates and momenta is given by the Hamiltonian equation:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{x}}, \qquad \frac{d\mathbf{x}}{dt} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} \tag{1}$$

Here $\mathcal{H}$ is the Hamiltonian function, $\mathbf{x}$ is a vector that consist of all the general coordinates, $\mathbf{p}$ is the conjugate momentum vector.[1] Classical mechanics is invariant under time reversal. Performing the time reversal transformation ($t \to -t$) also reverses the momenta ($\mathbf{p} \to -\mathbf{p}$) and the transformation leaves the Hamiltonian equation unchanged. If $\mathbf{x}_t$ is the coordinate of all the particles at time t, then the time-reversed motion is given by the curve $\mathbf{x}_{-t}$, in which the same positions occur in the reverse order. The time-reversed trajectory can be obtained by reversing the momentum of all the particles of the system. For every trajectory that satisfies the Hamiltonian equation, the time-reversed trajectory also satisfies the Hamiltonian equation.[2]

The time evolution of many mechanical systems is very sensitive to the initial conditions. In such systems, two initially infinitesimally close trajectories that start from the points $(\mathbf{x}_0, \mathbf{p}_0)$ and $(\mathbf{x}_0, \mathbf{p}_0) + \delta(\mathbf{x}_0, \mathbf{p}_0)$ in the phase space diverge exponentially fast. The Lyapunov exponent λ provides a direct measure of the rate of separation between the trajectories.[3, 4].

$$\frac{d}{dt}\delta(\mathbf{x}_t, \mathbf{p}_t) = \lambda \cdot \delta(\mathbf{x}_t, \mathbf{p}_t) \tag{2}$$

Here $\delta(\mathbf{x}_t,\mathbf{p}_t)$ is the distance between the two trajectories at time t.

Macroscopic objects consist of a large number of microscopic particles. It has been shown that the microscopic dynamics of the particles has positive Lyapunov exponent, thus these systems exhibit strong dependence on the initial conditions.[5]

Macroscopic thermodynamic systems spontaneously evolve towards future equilibrium states, but they do not spontaneously evolve away from equilibrium. The second law of thermodynamics, which says that the entropy of an isolated system never decreases, postulates this time asymmetry. A statistical interpretation of entropy can be given using the probabilities of microscopic states of the system.[6]

$$S=-k_B\cdot\int\rho(\mathbf{x},\mathbf{p})\cdot\ln\left(\rho(\mathbf{x},\mathbf{p})\right)\cdot d\mathbf{x}d\mathbf{p} \qquad (3)$$

Here S is the entropy of the system, the integral is over all the microstates that can realise the observed macrostate of the system, $\rho(\mathbf{x},\mathbf{p})$ is the probability density function of the microstates corresponding to the macrostate of the system, k_B is the Boltzmann constant. Entropy is a property of the macrostate, not of the microstate. The entropy introduced above expresses our uncertainty about the microscopic state of the system, if the macroscopic state is known, but no microscopic information is available.

Efforts to reconcile the irreversibility of thermodynamics with the reversibility of the underlying microscopic dynamics led Boltzmann to the famous H-theorem almost one and a half century ago.[7] More recently, fluctuation theorems were derived [8-10] and tested in several experiments.[11-14] Lifting the requirement for the thermodynamic limit, these theorems provide a generalisation of the second law of thermodynamics to small systems far from equilibrium. Both the H theorem and the fluctuation theorems predict entropy increase for macroscopic isolated systems. Other theories assume that time is a discrete quantity[15, 16], make assumptions about the initial state of the Universe [17] or about the energy and momentum of the system [18] to arrive to the second law of thermodynamics, or imply a

Universe that is statistically time symmetric on ultra large scales.[19] Deriving the second law of thermodynamics from the laws of mechanics is still an open question.[20]

All “derivations“ of the second law of thermodynamics suffer from at least one of the following two unsolved problems. First, they introduce time-asymmetry through extra assumptions in addition to the laws of mechanics so they fail to derive the laws of thermodynamics only from mechanics. Second, they cannot distinguish between the forward and backward directions of time. There is no directionality of time in the equations of microscopic mechanics, nor in the reasoning used in these derivations. The proofs could be done the same way backwards also, extrapolating from later to earlier times. This would predict larger entropy for earlier times, which is in disagreement with the observations.[9] One may argue that extrapolating backwards in time is unnatural, but it seems unnatural only if we assume that the two directions of time are not equivalent, which is exactly what we would like to show.

Computer simulations also show an increase of entropy for isolated systems, but they also result in larger entropies if calculating backwards in time, thus predicting entropy decrease in the past, which is in contradiction with the observations.

In 1929 Edwin Hubble observed that the recession velocity (v) of distant galaxies is roughly proportional to their distance from Earth (r) [21, 22]

$$v = H_0 \cdot r \tag{4}$$

The proportionality constant $H_0 = 67.8 \pm 1.2 (km/s)/Mpc \approx 2.2 \cdot 10^{-18} s^{-1}$ is called Hubble's parameter.[23] The cosmological explanation offered by general relativity for Hubble’s observation is that space itself is expanding, which affects the positions and momenta of objects.

According to the theory of general relativity, gravity is not a force, but rather a property of space-time. The Einstein field equation connects the curvature of space-time described by the Einstein tensor ($\mathbf{G}_{\alpha\beta}$) with the stress-energy tensor ($\mathbf{T}_{\alpha\beta}$):

$$\mathbf{G}_{\alpha\beta} = \frac{8\pi G}{c^4} \cdot \mathbf{T}_{\alpha\beta} \tag{5}$$

Here G is Newton's gravitational constant, c is the speed of light in vacuum. The simple appearance of the Einstein field equation hides a complicated set of ten coupled nonlinear partial differential equations. Exact solutions were only found using simplifying assumptions.

Cosmology uses the Einstein field equation to describe the evolution of the Universe. The cosmological principle assumes that the Universe is homogeneous and isotropic on very large scales. These assumptions imply the existence of a universal time coordinate and the possibility of defining space at any time point as the three dimensional surface perpendicular to the time coordinate. The cosmological principle also narrows down the possible solutions of the Einstein field equation to only three options known as the Friedmann–Lemaître–Robertson–Walker (FLRW) metric:

$$ds^2 = -c^2dt^2 + a^2(t)\left[\frac{dr^2}{\left(1-Kr^2\right)} + r^2\left(d\theta^2 + \sin^2\theta d\phi^2\right)\right] \tag{6}$$

K is a constant representing the curvature of space, with possible values of -1, 0 or 1. The above metric describes an expanding Universe, in which expansion of space is accounted for by a time dependent dimensionless scale factor $a(t)$. The standard convention is to set $a(t)=1$ today. In the above equation t is cosmic time, which is the time measured by comoving observers who move together with the expansion of the Universe and stay at rest in the comoving coordinates r,θ,ϕ ($dr=0, d\theta=0, d\phi=0$). The Hubble parameter is the ratio of the rate of change of the scale factor to the current value of the scale factor [22]:

$$H(t) = \frac{\frac{da(t)}{dt}}{a(t)} \tag{7}$$

As we can see, the Hubble parameter also changes with time; H_0 is the value observable today. Whether and how metric expansion affects the dynamics of local systems is still an unsettled question. Early works on this subject found that simple symmetric systems could be embedded in the FLRW metric without being influenced by the expansion.[24] The FLRW metric, however, does not set a lower limit for the scale of the expansion. Recent calculations on more realistic systems concluded that the expansion affects all scales, but on small scales it remains undetectably small.[25-28]

Approximating space by Euclidean space is an excellent approximation everywhere except near black holes and on scales comparable to the size of the Universe. Assuming slow motions (v<<c), under Euclidean approximation the dynamics of interacting objects moving in a FLRW metric can be described using a pseudo-Newtonian model.[29-32] In this simplified model, the inertial reference frame of the expanding Universe is the comoving coordinate system. As derived in [31], other non-rotating reference frames move compared to the comoving frame with an instantaneous velocity of $H\mathbf{x}$ and acceleration of $\frac{\frac{d^2a}{dt^2}}{a}\cdot\mathbf{x}$. The coordinate transformation can be taken into account by transforming velocities and accelerations in the Newtonian model. The new equation of motion is [31]:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial U(\mathbf{x})}{\partial \mathbf{x}} + \frac{\frac{d^2a}{dt^2}}{a}\cdot\mathbf{x} \tag{8}$$

Where $U(\mathbf{x})$ denotes potential energy. The i-th component of the observed velocities can be calculated as [31]:

$$\frac{dx_i}{dt} = \frac{p_i}{2m_i} + H\cdot x_i \tag{9}$$

The expansion of the Universe introduces an inherent irreversibility, presenting a cosmological "arrow of time". Classical mechanics also introduces a time concept, but the equations of mechanics are time reversible, showing no directionality. The time asymmetry of thermodynamics establishes a thermodynamic "arrow of time".

Efforts to derive the laws of thermodynamics from mechanics and scientific debates around possible mechanistic explanations of the second law of thermodynamics date back to the 1860s.[7] With the development of cosmology, other questions were also formulated about the relationship between mechanics, cosmology and thermodynamics.

How does the reversible mechanics of the particles at the microscopic level result in the observed directionality of thermodynamics? What is the detailed microscopic background of the entropy increase of isolated systems? What is the connection between the thermodynamic and cosmological "arrow of time", if there is any? Can the expansion of the Universe affect significantly local phenomena? The above questions are at the foundation of science, but no satisfactory answers were found yet. Here I use a new approach to answer these questions.

This paper derives thermodynamic irreversibility applying only the laws of classical mechanics and the expansion of the Universe to multi-particle systems, without any extra assumptions.

2. Results and Discussion

2.1. Could metric expansion of the Universe influence dynamics on small scales?

Metric expansion has been used to describe the large scale structure of the Universe. However, the theory has no built-in size limit. The cosmological redshift of the background electromagnetic radiation affects all wavelengths indicating that short lengths are also changed by the metric expansion. The effect of metric expansion of the Universe is undetectably small on shorter scales than the distance between galaxies.[25-28] This paper shows that if the expansion of the Universe has any – even immeasurably small – contribution to the local metric, that can give rise to the irreversibility observed in thermodynamic systems.

Atoms of everyday objects do not move freely along geodesics, because they are bound by electromagnetic forces. This does not allow objects to visibly expand, but metric expansion causes a small change in the phase space trajectory of bound systems.[30-32] The expansion of the Universe thus displaces the point describing the system in the phase space. This displacement is so small that it remains undetectable in systems that do not amplify the small deviation from the reversible Hamiltonian trajectory thus we observe reversible mechanics. In thermodynamic systems, which consist of many particles, however, the small departure from the original path increases exponentially due to the strong sensitivity to the initial conditions. The system will reach microscopic states that are far from the microstates expected based on the Hamiltonian equation. The characteristic timescale of the separation between the two microscopic trajectories is determined by the Lyapunov exponent, which is in the order of $10^{10}s^{-1}$ in air and $10^{12}s^{-1}$ in water.[33] The initial deviation from the reversible mechanics is thus exponentially amplified with characteristic times, in the order of $10^{-12}-10^{-10}s$.

2.2. Applying the expansion of the Universe to small distances assuming FLRW metric

Let us consider an isolated thermodynamic system that consists of N elastically colliding particles. Under such conditions, no external interactions change the entropy of the system. Let us assume further that this thermodynamic system is in a region where the expansion of the Universe can be described by the FLRW solution, space can be approximated by Euclidean space, and the particles that build up the system move much slower than the speed of light. In this case, the microscopic dynamics of the particles can be described by the following equation [31]:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial U(\mathbf{x})}{\partial \mathbf{x}} + \frac{\frac{d^2 a}{dt^2}}{a}\mathbf{x} \tag{10}$$

$$\frac{dx_i}{dt} = \frac{p_i}{2m_i} + H \cdot x_i \tag{11}$$

The $H \cdot x_i$ term breaks the time symmetry of the equation. The time reversal transformation ($t \to -t$) results in:

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial U(\mathbf{x})}{\partial \mathbf{x}} + \frac{\frac{d^2 a}{dt^2}}{a}\mathbf{x} \tag{12}$$

$$\frac{dx_i}{dt} = \frac{p_i}{2m_i} - H \cdot x_i \tag{13}$$

To leave the equation unchanged, time reversal has to be combined with changing the expansion of the Universe to contraction, with the Hubble constant $H \to -H$. To see a system go through the same positions in backwards order it is not enough to reverse the momentum of all particles, the expansion of the Universe would need to be reversed also.

The time evolution plotted out by the new equation has a non-zero divergence in the phase space. For isolated systems the divergence of the time evolution can be calculated as:

$$\Lambda = div\left(\frac{d\mathbf{x}}{dt}; \frac{d\mathbf{p}}{dt}\right) = \sum_{i=1}^{3N}\left(\frac{\partial}{\partial x_i}\cdot\frac{dx_i}{dt} + \frac{\partial}{\partial p_i}\cdot\frac{dp_i}{dt}\right) \tag{14}$$

Using equation (10) and (11) we obtain:

$$\Lambda = \sum_{i=1}^{3N}\left(\frac{\partial}{\partial x_i}\cdot\left(\frac{p_i}{2m_i} + H \cdot x_i\right) + \frac{\partial}{\partial p_i}\cdot\left(-\frac{\partial U(\mathbf{x})}{\partial \mathbf{x}} + \frac{\frac{d^2 a}{dt^2}}{a}\mathbf{x}\right)\right) = \sum_{i=1}^{3N}(H) = 3 \cdot N \cdot H \tag{15}$$

Neglecting the change of the Hubble constant we obtain:

$$\Lambda \approx 3 \cdot N \cdot H_0 \tag{16}$$

2.3. Time scale on which irreversibility arises in thermodynamic systems

We have seen that metric expansion causes a small deviation from the trajectory expected based on the reversible Hamiltonian mechanics. This deviation then is amplified by the dynamics of the particles in systems that have positive Lyapunov exponent. Let us give an upper estimate for the time in which the departure of the actual trajectory from the trajectory expected based on the Hamiltonian equation becomes important. The distance between the two trajectories has components on both the momenta and the coordinates. If the two trajectories diverged in the space coordinates, they also diverged in the phase space. To keep the calculations simple let us consider only the distance in the space coordinates between the two trajectories. If we start to follow the time evolution of a system at time t_0, and denote the deviation between the two trajectories in space by $\delta\mathbf{x}(t)$, then we can write:

$$\frac{d}{dt}\delta\mathbf{x}(t) = \lambda \cdot \delta\mathbf{x}(t) + H_0 \cdot \mathbf{x}(t) \tag{17}$$

Solving the differential equation we get:

$$\delta\mathbf{x}(t) = H_0 \cdot e^{\lambda\cdot(t-t_0)} \cdot \int_{t_0}^{t} \mathbf{x}(t') \cdot e^{-\lambda\cdot(t'-t_0)} dt' \tag{18}$$

On the right hand side of the above equation $H_0 \approx 2.2\cdot 10^{-18} s^{-1}$, $\lambda \approx 10^{12} s^{-1}$ in water and $\lambda \approx 10^{10} s^{-1}$ in air [33], the integral can be approximated as $\mathbf{x}/\lambda \approx \mathbf{x}\cdot 10^{-12} s$ in water and $\mathbf{x}/\lambda \approx \mathbf{x}\cdot 10^{-10} s$ in air. Based on the above calculation, $\delta\mathbf{x}$ would become comparable to $\mathbf{x}$ in $\approx$ 68 ps in water and in $\approx$ 6.4 ns in air. The time in which microscopic irreversibility arises due to the metric expansion of the Universe is in fact shorter than the value calculated above. The linear relationship between $\frac{d}{dt}\delta\mathbf{x}(t)$ and $\delta\mathbf{x}(t)$ only holds for small deviations. If the deviation between the two trajectories becomes important for the dynamics of the system, the linear dependence breaks down. This will happen earlier than the times calculated above, so these calculations provide an upper limit for the time in which expansion of the Universe affects significantly the state of a thermodynamic system.

2.4. Entropy increase

Let us consider again an isolated system that starts to evolve from time t_0 and an initial microstate $(\mathbf{x}_0, \mathbf{p}_0)$. This microstate corresponds to a macroscopic state, which implies a probability density function of the microstates $\rho(\mathbf{x}_0, \mathbf{p}_0)$. After a short time t, which is shorter than the characteristic Lyapunov time $1/\lambda$, the system will be in the $(\mathbf{x}_t, \mathbf{p}_t)$ state. Metric expansion causes a small deviation from the Hamiltonian path resulting in a state with slightly different entropy than expected based on the Hamiltonian evolution. For times much shorter than $1/\lambda$, metric expansion of space gives a small correction to the Hamiltonian time evolution of the system. The entropy difference between the distributions belonging to the Hamiltonian and the true time evolutions can be calculated:

$$\Delta S \approx k_B \cdot (t - t_0) \cdot \int \rho(\mathbf{x}_0, \mathbf{p}_0) \cdot \Lambda \cdot d\mathbf{x}_0 d\mathbf{p}_0 \tag{19}$$

We know that $\Lambda \approx 3 \cdot N \cdot H_0$, and that the integral of the density function over the entire phase space is 1, thus:

$$\Delta S \approx k_B \cdot (t - t_0) \cdot N \cdot H_0 \tag{20}$$

The above expression is always positive. This means that the direction of the deviation from the Hamiltonian path due to FLRW expansion is always towards an entropy increase. Small random disturbances arising from unavoidable interactions with the environment cannot result in a similar systematic entropy increase. Such disturbances divert the microscopic evolution of the system between different Hamiltonian trajectories with the same probability in one direction and backwards, thus such disturbances cannot introduce a preference for entropy increase.

The FLRW metric describes the expansion of the Universe on very large scales on which the Universe can be considered homogeneous. The metric is not FLRW near massive objects. Here the metric can be determined by taking into account both the nearby masses and the overall expansion of the Universe. The nonlinearity of general relativity makes the calculation of the resulting metric difficult. We know that the metric is dominated by the nearby mass, but it should also contain a small contribution from the entire Universe. For our explanation of irreversibility in thermodynamic systems it practically does not matter how small the contribution from the expansion of the Universe is. In systems with positive Lyapunov exponent, any small contribution from the metric expansion couples the local dynamics of the system to the evolution of the Universe. In these systems, the small perturbation arising from the expansion of the Universe increases exponentially. Let us assume for a moment that the perturbation that arises from the expansion of the Universe is $e^7 \approx 1000$ times smaller than the effect that would come from the FLRW metric. In this case, the time in which macroscopic irreversibility arises due to the expansion of the Universe would increase by ≈ 7 ps in water and ≈ 0,7 ns in air compared to the one calculated based on the FLRW metric, because initial perturbations increase by a factor of e every 1 ps in water and 0,1 ns in air. In this situation irreversibility would arise in maximum 75 ps in water and 7,1 ns in air, compared to the 68 ps in water and 6,4 ns in air calculated using FLRW metric.

We know that the Hubble "constant" has changed during the history of the Universe. This, however, does not affect our explanation. The time in which irreversibility becomes visible is mostly determined by the dynamics of the system (Lyapunov exponent), and not by the Hubble parameter of the expansion of the Universe. The expansion of the Universe only provides a small initial perturbation. This picture would change only if the coefficients of the first and second term on the right hand side of eq. 17 become comparable. For the studied example of water $\lambda \approx 10^{12} s^{-1}$. The term containing the Hubble parameter becomes comparable to the dynamic term only with a Hubble parameter which is 10^{30} times larger than the one observed today. Assuming that the Hubble parameter changed inversely proportional with cosmic time, this happened only in the very early life of the Universe, roughly when the size of the Universe was smaller than $10^{-4}m$. In this realm, however, all the assumptions of mechanics also brake down.

3. Conclusions

This paper shows that the time asymmetry of thermodynamics could be explained based on the effect of the expansion of the Universe on local mechanics, without any extra assumptions. Ilya Prigogine believed that the second law of thermodynamics had a dynamical origin. He argued that the microscopic dynamics is inherently irreversible. This paper gives a possible explanation of the origin of the microscopic irreversibility assumed by Prigogine.

Based on the thoughts presented above we are able to answer the questions raised earlier.

Can the expansion of the Universe affect significantly local phenomena? Yes, metric expansion of space can be important in systems with positive Lyapunov exponents.

How does the reversible mechanics of the particles at the microscopic level result in an irreversible thermodynamics on the macroscopic scale? Mechanics is not completely reversible as a result of the metric expansion of space, which causes a time asymmetry in the evolution of thermodynamic systems.

What is the detailed microscopic background of the entropy increase of isolated systems? It has been shown for a simplified case (approximating space by Euclidean space, assuming slow motions (v<<c) and Friedmann–Lemaître–Robertson–Walker metric) that metric expansion of space results in a constant departure from the Hamiltonian evolution towards states with larger entropy in isolated systems.

What is the connection between the thermodynamic and cosmological "arrow of time", if there is any? Expansion of the Universe causes a small displacement in the phase space trajectory of thermodynamic systems. The small displacement is amplified exponentially in time by the microscopic dynamics of the particles in systems with positive Lyapunov exponent, causing macroscopically detectable irreversibility. The evolution of thermodynamic systems is thus visibly coupled to the evolution of the Universe in a very short time. In this sense, the cosmological "arrow of time" can be considered a "master arrow of time", which implies the "thermodynamic arrow of time".

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