Verschränkung versus Stosszahlansatz: Disappearance of the Thermodynamic Arrow in a High-Correlation Environment

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The crucial role of ambient correlations in determining thermodynamic behavior is established. A class of entangled states of two macroscopic systems is constructed such that each component is in a state of thermal equilibrium at a given temperature, and when the two are allowed to interact heat can flow from the colder to the hotter system. A dilute gas model exhibiting this behavior is presented. This reversal of the thermodynamic arrow is a consequence of the entanglement between the two systems, a condition that is opposite to molecular chaos and shown to be unlikely in a low-entropy environment. By contrast, the second law is established by proving Clausius' inequality in a low-entropy environment. These general results strongly support the expectation, first expressed by Boltzmann and subsequently elaborated by others, that the second law is an emergent phenomenon that requires a low-entropy cosmological environment, one that can effectively function as an ideal information sink.

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The status of the second law of thermodynamics and the emergence of macroscopic irreversibility from time-symmetric dynamical laws have been widely debated since Boltzmann's ground breaking work relating thermodynamic behavior to microscopic dynamics late in the nineteenth century. Indeed, rarely have so many distinguished physicists written as extensively on a subject while achieving so little consensus. The debate continues to present day, having gained intensity in recent decades as a surge of activity in such topics as chaos, quantum computing, and quantum information theory has stimulated interest in the subject [1].

There is nevertheless a slowly growing consensus that the asymmetry observed in macroscopic phenomena originates in the "initial conditions" of our cosmic neighborhood, and ultimately that of the whole universe. Remarkably, Boltzmann himself arrived at the hypothesis that "the universe, considered as a mechanical system—or at least a very large part of it which surrounds us—started from a very improbable state, and is still in a very improbable state" as the initial condition that was required to explain the asymmetry in the second law [2]. This view has subsequently been echoed by Gold, Feynman, Lebowitz and coworkers, Peierls, Penrose, and others [3], albeit with various degrees of emphasis and detail. In particular, Penrose has characterized the improbability of the initial state of the universe by the vanishing of the Weyl tensor in the early, homogeneous universe, in contrast to its preponderance in the final, clumped stages (which are the higher entropy states in the presence of gravity). If so, how is the influence of a low-entropy, time-asymmetric cosmological environment felt by a thermodynamic system? "This is reflected in Boltzmann's *stosszahlansatz*," remarks Peierls [3], referring to Boltzmann's assumption of molecular chaos that single particle states are uncorrelated in a dilute gas [4]. Presumably, one would expect the initial correlations among the molecules of the gas to be small in a low-entropy environment, thus allowing subsequent interactions to raise their individual entropies toward equilibrium.

Thus arises the question of whether in a high-entropy environment interactions can lower initially high correlations among the molecules, thereby lowering their individual entropies and reversing the thermodynamic arrow. More specifically, can the direction of heat flow be reversed in an environment in which entanglement is more typical than molecular chaos? The primary purpose of this Letter is to show that this is indeed possible. In particular, we construct a class of entangled states of two macroscopic systems such that each individual component is in a state of thermal equilibrium at a given temperature, and when the two are allowed to interact heat can flow from the colder to the hotter system. An explicit example of this class where the two systems are dilute gases is also constructed. The resulting reversal of the thermodynamic arrow is thus a consequence of entanglement between the two systems. In effect, this entanglement disables the statistical biases that give rise to normal thermodynamic behavior. To analyze the opposite scenario, we first establish the result that correlations are generally small in a low-entropy environment, a result that justifies the condition of generalized molecular chaos in a low-entropy universe. We then establish the second law by proving Clausius' inequality in a low-entropy environment. These results strongly support the view that the second law and the thermodynamic arrow are emergent phenomena that require a low-entropy environment, with the universe effectively functioning as an infinite information sink. In our cosmic neighborhood, this is made possible by a bright sun against a dark sky, thus maintaining a steady process of entropy disposal [5]. Needless to say, the currently favored accelerating models of big bang cosmology nicely accommodate the role required of the universe.

As a preliminary step, we will establish the result that two-body correlation is on average bounded by single-body entropy in any collection of $N \geq 3$ interacting systems. Let the systems be labeled $i = 1, 2, \ldots N$, and the corresponding von Neumann entropies S^i. To quantify two-body correlations, we will use $I^{ij} = S^i + S^j - S^{ij}$, the quantum measure of mutual information. The basic tool in the derivation is the strong subadditivity property of entropy in the form $S^i + S^j \leq S^{ik} + S^{jk}$ [6]. Since there are $N(N-1)/2$ distinct pairs in the collection, there will be as many distinct inequalities resulting from strong subadditivity. When aggregated, they give

$$[N(N-1)/2]^{-1} \sum_{i<j=1}^{N(N-1)/2} I^{ij} \leq N^{-1} \sum_{i=1}^{N} S^i. \quad (1)$$

Thus $I_{av} \leq S_{av}$, indicating that a small average entropy guarantees a low level of two-body correlations. The significance of this general result is the validity of Boltzmann's *stosszahlansatz*, for any two systems whether microscopic or macroscopic, as a likely condition in a low-entropy universe. Note that we established this result without any reference to such problematic issues as the purity level of the wavefunction of the universe.

In much of what follows, we will rely on a fundamental inequality that governs the evolution of any system whose initial state is one of thermal equilibrium. Let the initial and final states of the system be $\rho_i = \exp(-\beta H_i)/Z$ and ρ_f respectively, where $\beta = 1/k_B T$. Here ρ_i is the density matrix describing the initial Gibbs state, with H_i the initial Hamiltonian operator, Z the partition function, T the temperature, and k_B the Boltzmann constant. Note that the Hamiltonian may change during the evolution, causing exchange of work. Thus the final Hamiltonian H_f will in general be different from H_i. The evolution itself will in general not be unitary as it may involve interaction with other systems, and the final state ρ_f may not be one of equilibrium.

Now consider $S(\rho_f \| \rho_i)$, the relative entropy of ρ_f with respect to ρ_i, which is a non-negative quantity defined as $-S(\rho_f) - \mathrm{tr}(\rho_f \log \rho_i)$. The latter property can be used to establish that

$$S(\rho_f \| \rho_i) = \beta \Delta U - \Delta S - \beta \, \mathrm{tr}(\rho_f \Delta H) \geq 0, \quad (2)$$

where $\Delta U = U_f - U_i = \mathrm{tr}(\rho_f H_f) - \mathrm{tr}(\rho_i H_i)$, $\Delta S = S_f - S_i$, and $S(\rho) = -\mathrm{tr}(\rho \log \rho)$ is the von Neumann entropy. It is important to realize that this inequality stipulates an *initial* equilibrium state and temperature only, and as such is fundamentally different from the standard inequalities of equilibrium thermodynamics.

Verschränkung versus *Stosszahlansatz*. Consider two systems A and B, each individually in thermal equilibrium at temperatures β^A and β^B initially, which are placed in thermal contact and allowed to exchange heat but not work. In that case $\Delta H = H_f - H_i = 0$, ΔU equals the absorbed heat Q, and inequality (2) reduces

to $\beta Q - \Delta S \geq 0$ [7]. Applying the latter to each of the two systems in the above process, we find $\beta^A Q^A \geq \Delta S^A$ and $\beta^B Q^B \geq \Delta S^B$, while $Q^A + Q^B = 0$. We will next apply these inequalities to the extreme cases of zero and maximum initial correlations, designating them as cases **S** and **V** respectively.

Case S. If the two systems are initially uncorrelated, as is typically expected in a low-entropy environment according to (1), we will have $\rho_i^{AB} = \rho_i^A \otimes \rho_i^B$ and $S_i^{AB} = S_i^A + S_i^B$. On the other hand, the final state ρ_f^{AB} will generally be correlated due to the interaction and we will have $S_f^{AB} \leq S_f^A + S_f^B$. Since the two systems interact in isolation from the rest of the universe, ρ_i^{AB} and ρ_f^{AB} will be related unitarily and we have $S_f^{AB} = S_i^{AB}$, which in conjunction with the foregoing relations leads to $\Delta S^A + \Delta S^B \geq 0$. Combining the latter with the inequalities of the preceding paragraph, we find $\beta^A Q^A + \beta^B Q^B \geq 0$. Since $Q^A + Q^B = 0$, the last inequality implies that Q^A has the same sign as $\beta^A - \beta^B$ or $T^B - T^A$, i.e., that heat flows from the *initially* hotter system to the *initially* colder one. This is of course a fundamental law of nature, and is seen here to follow where generalized *Stosszahlansatz* holds. In essence, the foregoing argument reflects Boltzmann's original reasoning: starting from an uncorrelated initial configuration, there are overwhelmingly more possibilities for final states if the initially colder state gains energy than vice versa. Model calculations using molecules as interacting thermodynamic systems verify this expectation in detail [7].

Case V. The above scenario changes dramatically if the two interacting systems are significantly correlated to begin with, as may be expected in a high-correlation environment [8]. To demonstrate this assertion, we will consider the extreme case where the two systems are initially entangled in a pure state while each individual system is in thermal equilibrium. These conditions can be realized for a pair of macroscopic systems whose energy spectra, $\{E_i^A\}$ and $\{E_i^B\}$, are identical except for a scale factor, i.e., if $\mu^A E_i^A = \mu^B E_i^B = \epsilon_i$. The desired joint state of the two systems can then be represented as $\rho^{AB} = |\Omega^{AB}\rangle\langle\Omega^{AB}|$, with

$$|\Omega^{AB}\rangle = Z^{-1/2} \sum_i \exp(-\gamma \epsilon_i/2)|i; A\rangle|i; B\rangle, \quad (3)$$

where $|i; A\rangle$ ($|i; B\rangle$) is the ith energy eigenvector for system A (B), γ is a positive constant, and $Z^{-1/2}$ is a normalization constant. Note that Eq. (3) is essentially the Schmidt decomposition of $|\Omega^{AB}\rangle$. It can now be readily verified that the individual states of the two systems (obtained from ρ^{AB} by tracing over the Hilbert space of the other) are thermal equilibrium states at temperatures given by $\beta^A = \mu^A \gamma$ and $\beta^B = \mu^B \gamma$.

Just as in case **S**, we consider a process of heat exchange between A and B and find $\beta^A Q^A \geq \Delta S^A$, $\beta^B Q^B \geq \Delta S^B$, and $Q^A + Q^B = 0$. However, in contrast to case **S**, the joint state of the two systems is pure in

this case, so that ρ^A and ρ^B are now isospectral with the consequence that $S^A = S^B$ at all times and $\Delta S^A = \Delta S^B$ for the process. Since in general $Q^A Q^B \leq 0$, the above inequalities imply that $\Delta S^A = \Delta S^B \leq 0$, thus reversing the inequality we found for $\Delta S^A + \Delta S^B$ in case **S**. This reversal in turn leads to $\beta^A Q^A + \beta^B Q^B \geq \Delta S^A + \Delta S^B$, which allows both directions of heat flow, including that from the initially colder body to the hotter one. Note that equality in this result obtains only if there is zero heat exchange between the systems (in violation of the zeroth law since initial temperatures are unrestricted here). We will later present a model exhibiting this reversal explicitly.

What is the cause of this bizarre behavior? The clue is in the dual character of $|\Omega^{AB}\rangle$: while entanglement forces the individual entropies S^A and S^B to move in lock-step, the maximal entropy of the initial equilibrium states implies that the individual entropies can only decrease. Therefore, there is no opportunity for any statistical dominance of one direction of heat flow over the other, in stark contrast to case **S**. This feature is strikingly apparent in the model calculation considered later. The main lesson to be drawn here is that the statistical biases that cause normal thermodynamic behavior can be neutralized by pre-existing correlations between the interacting systems. Thus a low-entropy environment, which serves to guarantee low correlations and preclude the anomalous behavior just described, is indeed a prerequisite for normal thermodynamic behavior.

To further highlight the contrast between the two cases considered above, we will now establish the second law in case **S** by proving Clausius' Theorem in a low-entropy environment. Consider a macroscopic system that undergoes a cyclic evolution in thermal contact with a series of heat reservoirs, absorbing Q_j^S from the reservoir at temperature T_j^R while exchanging work as a result of possible changes in its Hamiltonian (e.g., because of expansion). Note that by definition the work exchange is associated with a unitary evolution and does not entail information transfer, in contrast to the heat exchange with the reservoir. Note also that T_j is the temperature of the jth reservoir, as there's no presumption of thermal equilibrium with the system here.

Consider the jth process, starting with the uncorrelated system-reservoir state $\rho_j^S \rho_j^R$, where ρ_j^R is a Gibbs state at temperature T_j^R and ρ_j^S is arbitrary, and culminating in the correlated state ρ_j^{SR}. The Hamiltonian operator governing this evolution may be represented as $H_j^S + V_j^S + H_j^R + H_j^{SR}$, where H_j^S and H_j^R refer to the system and reservoir, H_j^{SR} to their interaction, and V_j^S to the interaction of the system with the external agents with which it is exchanging work. Just as in case **S** above, we find $\Delta S_j^S + \Delta S_j^R \geq 0$, V_j^S notwithstanding, and applying inequality (2) to the *reservoir*, we conclude that $\beta_j^R Q_j^R \geq \Delta S_j^R$, where $\beta_j^R = 1/kT_j^R$ refers to the initial

temperature of the reservoir. Furthermore, the energy exchange between the system and the reservoir is subject to $Q_j^R = -Q_j^S$, since the work exchange does not involve the reservoir. Combining the last two inequalities, we find $\beta_j^R Q_j^S + \Delta S_j^S \leq 0$. Remarkably, the system obeys this inequality without necessarily having a well-defined temperature (β_j^R refers to the reservoir) and regardless of possible changes in its Hamiltonian.

If the last inequality is summed over the cycle, the entropy changes add up to zero, since the final state of the system is the same as the initial one, and we find

$$\sum_j \beta_j Q_j^S \leq 0, \tag{4}$$

which is Clausius' inequality.

Next we will construct a dilute-gas model for case **V** that will exhibit heat flow from the colder to the hotter system. The dilute nature of the two gases allows us to simplify the calculation by focusing attention on single particle interactions. We therefore consider particle a of one gas interacting with particle b of the other in a volume V. The initial, joint state of the two is pure and entangled, but in such a way that their individual states are in thermal equilibrium at different temperatures. To exhibit the structure of this state, we let $|a, \alpha_a \mathbf{k}\rangle$ represent a state of momentum $\alpha_a \mathbf{k}$ for particle a and $|b, \alpha_b \mathbf{k}\rangle$ a state of momentum $\alpha_b \mathbf{k}$ for particle b, where α_a and α_b are positive parameters. The joint state of the two particles is then

$$|\omega^{ab}\rangle = Z^{-1/2} \sum_{\mathbf{k}} \exp(-\gamma \mathbf{k}^2/4m)|a, \alpha_a \mathbf{k}\rangle|b, \alpha_b \mathbf{k}\rangle, \tag{5}$$

where Z and γ are as defined in Eq. (3), m is a mass scale, and we have set $\hbar = 1$.

It is useful at this point to continue the calculation using the configuration representation in the infinite-volume limit. Then Eq. (5) appears as

$$\omega^{ab}(\mathbf{r}^a, \mathbf{r}^b) = [\sqrt{Z}(2\pi)^3]^{-1} \int d^3k \exp(-\gamma \mathbf{k}^2/4m)$$
$$\times \exp(i\alpha_a \mathbf{k} \cdot \mathbf{r}^a) \exp(i\alpha_b \mathbf{k} \cdot \mathbf{r}^b). \tag{6}$$

The individual (or marginal) states of the two systems can now be found as

$$\rho^a(\mathbf{r}, \mathbf{r}') = [Z(2\pi\alpha_a\alpha_b)^3]^{-1} \int d^3k \exp(-\gamma \mathbf{k}^2/2m\alpha_a^2)$$
$$\times \exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')], \tag{7}$$

and an analogous expression for ρ^b. Note that $\gamma \mathbf{k}^2/2m\alpha_a^2 = \beta^a \mathbf{k}^2/2m^a$, which identifies ρ^a as a Gibbs state at temperature $T^a = (k_B \beta^a)^{-1} = m\alpha_a^2/\gamma k_B m^a$, and similarly for ρ^b with $T^b = m\alpha_b^2/\gamma k_B m^b$, where m^a and m^b are the respective masses. Thus each system, if experimented upon in isolation from the other, will be found to be in thermal equilibrium at the specified temperature. However, if the two systems are allowed to interact, it is the pure state given in Eq. (6) that must be considered as their initial state.

To model a thermal interaction between the two systems, we consider an adiabatic switching of the interaction so that the initial and final states are non-interacting and the interaction of the two with external systems is made negligible. Such an interaction amounts to a collision, with $\omega^{ab}(\mathbf{r}^a, \mathbf{r}^b)$ representing the non-interacting incoming state. Therefore, the fully interacting state of the two-body system can be represented as

$$\omega_{int}^{ab}(\mathbf{r}^a, \mathbf{r}^b) = [\sqrt{Z}(2\pi)^3]^{-1} \int d^3k \exp(-\gamma \mathbf{k}^2/4m) \times \psi_{\mathbf{k}}^{+}(\mathbf{r}^a, \mathbf{r}^b), \tag{8}$$

where $\psi_{\mathbf{k}}^{+}(\mathbf{r}^a, \mathbf{r}^b)$ is the "in" state that corresponds to the non-interacting state $\exp(i\alpha_a \mathbf{k} \cdot \mathbf{r}^a)\exp(i\alpha_b \mathbf{k} \cdot \mathbf{r}^b)$. Note that the initial momenta of the particles in each term of the coherent superposition $\omega_{int}^{ab}(\mathbf{r}^a, \mathbf{r}^b)$ are collinear and proportional in magnitude, reflecting the entangled nature of this state. It is important to realize that there would be no such correlation between the initial momenta of the particles otherwise. For example, the uncorrelated initial state $\rho^a \otimes \rho^b$, which would be typical in a low-entropy environment and exhibit normal thermodynamic behavior as shown above for case **S**, entails particle pairs of uncorrelated momenta.

The correlation between the initial momenta of the colliding particles in $\omega_{int}^{ab}(\mathbf{r}^a, \mathbf{r}^b)$ makes it possible to determine the direction of energy flow from conservation laws. For a collision event that starts with momenta $\alpha_a \mathbf{k}$ and $\alpha_b \mathbf{k}$, we find that the fractional kinetic energy gain for particle a as a result of the collision is given by $4x(x-1)\sin^2(\theta/2)$, where $x = [m^a/(m^a + m^b)][(\alpha_a + \alpha_b)/\alpha_a]$, and θ is the scattering angle in the center-of-mass system. Thus for all but forward scattering, particle a gains energy if $x > 1$. This condition can be satisfied if $(m^a/m^b)(T^b/T^a) > 1$, where we have eliminated $\alpha_{a,b}$ in favor of the initial temperatures. Clearly, if $m^a > m^b$, particle a can gain energy even if $T^a > T^b$, thus reversing the normal direction of heat flow. Note that the direction of energy flow would then be the same for every term in the wave packet of Eq. (8), clearly indicating that thermal statistics play no role in this result. This is the main lesson of this example, to wit, that entanglement is capable of destroying normal thermodynamic behavior by defeating the statistical biases that underlie it, instead rendering such macroscopic outcomes as the direction of heat flow dependent on microscopic details.

We close this Letter with a few concluding remarks. First, we have focused on the two extremes of ambient correlations, cases **S** and **V**, primarily to underscore the contrast in their resulting thermodynamic behavior. To be sure, these extreme cases are idealizations. However, they do serve to characterize likely thermodynamic behavior under the specified conditions of ambient correlations. Second, while we have used the von Neumann

entropy extensively in our calculations, the main results of our analysis concern energy flow and are not committed to any specific interpretation of that quantity for non-equilibrium states. Rather, the primary role of the entropy function in our analysis is as a measure of information, which is inextricably intertwined with energy flow in thermodynamic interactions. Third, it may be noted that the results presented here apply to the thermodynamics of microscopic systems as well. However, the two regimes are distinguished by the magnitude of fluctuations, which are comparable to averages for microscopic systems and normally negligible for macroscopic systems. Finally, it is important to note the importance of using the quantum description where entanglement effects play an essential role. Thus we have avoided classical phase space methods as inadvisable in the present context, although it may be possible to formulate some of the arguments presented here in classical terms.

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[1] The literature on this subject can be traced through J. L. Lebowitz, Rev. Mod. Phys. **71**, S346 (1999), and A. Wehrl, *ibid.* **50**, 221 (1978); see also *Quantum Limits to the Second Law*, ed. D. P. Sheehan (AIP Conf. Proc. 643, 2002). Diversity of view, on the other hand, is evident in published letters, Phys. Today **47**, 11 (1994), written in reaction to J. L. Lebowitz, *ibid.* **46**, 32 (1993), as well as in J. Bricmont, Ann. (N.Y.) Acad. Sci. **79**, 131 (1996).

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