A Physical Basis for the Second Law of Thermodynamics: Quantum Nonunitarity

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Abstract: It is argued that if the non-unitary measurement transition, as codified by Von Neumann, is a real physical process, then the 'probability assumption' needed to derive the Second Law of Thermodynamics naturally enters at that point. The existence of a real, indeterministic physical process underlying the measurement transition would therefore provide an ontological basis for Boltzmann's *Stosszahlansatz* and thereby explain the unidirectional increase of entropy against a backdrop of otherwise time-reversible laws. It is noted that the Transactional Interpretation (TI) of quantum mechanics provides such a physical account of the non-unitary measurement transition, and TI is brought to bear in finding a physically complete, non-*ad hoc* grounding for the Second Law.

Keywords: Second Law of Thermodynamics; irreversibility; entropy; H-Theorem; transactional interpretation; wave function collapse.

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1. Introduction

Irreversible processes are described by the Second Law of Thermodynamics, the statement that entropy S can never decrease for closed systems: $\frac{dS}{dt} \geq 0$. This law is corroborated ubiquitously at the usual macroscopic level of experience. However, there remains great uncertainty and debate regarding exactly how it is that these commonplace irreversible processes arise from an ostensibly time-reversible level of description. Specifically, it is commonly assumed that the quantum level obeys only the unitary dynamics of the time-dependent Schrödinger equation, which is time-reversible. In addition, classical mechanics can be obtained as the small-wavelength limit of the quantum evolution, as Feynman showed in his sum-over-paths approach [1]. So where does the observed macroscopic irreversibility enter?

Boltzmann famously introduced irreversibility into his "H-theorem," an attempted derivation of the Second Law, through his *Stosszahlansatz* (assumption of molecular chaos)[2]. This assumption consists of treating molecular and atomic state transitions as stochastic and independent, such that the joint probabilities applying to the state transitions in any given interaction are taken as equal to the product of the individual probabilities. At the quantum level, the same sort of statistical independence arises in 'master equations' specifying the changes in the probabilities of occupation of states of the interacting micro-systems comprising a macroscopic system of interest.

Thus the irreversibility in both the quantum and classical cases arises due to the presence of the *Stosszahlansatz* in various forms. The latter has rightly been questioned as a circular, question-begging way of obtaining irreversibility (e.g., [3]). Meanwhile, Sklar has noted that "[t]he status and explanation of the initial probability assumption remains the central puzzle of non-equilibrium statistical mechanics"[4]. However, if there is a real, lawlike (even if indeterministic) physical origin for this statistical description of the state transitions of component systems, then the second law follows nomologically and non-circularly. Such a model will be presented herein. First, however, let us briefly review the basic problem.

2. Reversible vs non-reversible processes

Classical laws of motion are in-principle reversible with respect to time. There is a one-to-one relationship between an input *I* and an output *O*, where *I* and *O* are separated by a time interval Δt. If Δt is taken as positive, then *I* is the cause and *O* is the effect. If we reverse the sign of Δt, then the roles of the output and input are simply exchanged; the process can just as easily run backwards as forwards. The same applies to quantum processes described by the Schrödinger equation: the input and output states are linked in a one-to-one relationship by deterministic, unitary evolution.

Moreover, it is well established that the 'statistical operator' (density operator), ρ, applying to a quantum system obeys a unitary, time reversible dynamics, analogous to the Liouville equation for the phase space distribution of microstates in classical statistical mechanics. The general definition of the density operator (applying either to a pure or mixed state) is:

$$\rho = \sum_i P_i |\Psi_i\rangle\langle\Psi_i| \qquad (1)$$

where P_i is the probability that the system is in the pure state $|\Psi_i\rangle$, and the P_i sum to unity. The states $|\Psi_i\rangle$ need not be orthogonal, so in general $\{|\Psi_i\rangle\}$ is not a basis.

From the Schrödinger equation and its adjoint, ones finds the time-evolution of ρ :

$$\frac{\partial\rho}{\partial t} = \frac{-i}{h}[H,\rho] \qquad (2)$$

where H is the Hamiltonian. It is important however to note that ρ is not an observable; this is reflected in the sign difference between its time dependence and that of an observable *O,* which obeys $\frac{\partial O}{\partial t} = \frac{i}{h}[H,O]$. Significantly, ρ is defined independently of any particular basis. It must be distinguished from the so-called "density matrix," which we'll represent here by $\tilde{\rho}$. The latter is a particular *representation* of the density operator with respect to a given basis.

In contrast, non-unitary evolution such as that described by von Neumann's "Process 1," or measurement transition, is indeterministic [5]. An input state *I* is transformed to one of many possible output states O_i, elements of a particular basis, with no causal mechanism describing the occurrence of the observed output state O_k.[1] The different possible outcomes are statistically weighted by probabilities according to the Born Rule. As a result of the measurement transition, the system is represented by a density matrix $\tilde{\rho}$ as discussed above. This one-to-many transition is inherently irreversible; once a final state occurs, the original state is not accessible to it through simple time reversal.

However, the status of the non-unitary measurement transition has long been very unclear. It is commonly thought of as epistemic in nature—i.e., describing only a Bayesian updating of an observer's knowledge. Such an epistemic view of quantum measurement has its own interpretive problems, which we will not enter into here; but it also can provide no ontological basis for the observed asymmetry described by the Second Law.

On the other hand, if the measurement transition is a real (indeterministic) physical process, it is clearly a candidate for the ontological introduction of stochastic randomness--describable by

[1] Of course, hidden variables theories attempt to provide a causal mechanism by 'completing' quantum theory, but here we consider quantum mechanics as already complete and simply in need of a direct-action interpretation.

[2] As their names indicate, both of these objects are wavelike entities—specifically, they are deBroglie waves.

[3] However, TI is best understood in the Heisenberg picture, in which the observables carry the time dependence and the offer wave is static; this is to be discussed in a separate work.

probabilities such as those in master equations--and the resulting irreversibility described by the Second Law. In fact, Von Neumann himself showed that his 'Process 1' is irreversible and always entropy-increasing [5]. However, he seemed to have veered away from using that fact in deriving the Second Law, because he thought of the measurement transition as dependent on an outside perceiving consciousness, and as such not a real physical process.

3. Standard Approaches to the Second Law; "Smuggling In" Non-unitarity

A typical 'derivation' of the Second Law begins with unitary evolution to obtain the basic transition rates between various states, but ends up with a master equation from which one finds that the time rate of change in entropy is always positive (or zero for equilibrium). We'll consider this seeming paradox in what follows. First, recall that a master equation relates the change in the probability P_i that a system is in state $|i>$ to the transition rates R_{ij} between that state and other states $|j>$. Specifically:

$$\frac{dP_i}{dt} = \sum_j R_{ij}P_j - R_{ji}P_i \equiv [M]P_i \tag{3}$$

where [M] is the 'master operator.' Each diagonal element of [M] is the negative of the sum of all the off-diagonal elements in the same column (which are all positive). This property gives rise to a decaying exponential time-dependence, yielding an irreversible tendency to an equilibrium state, independently of the initial state of the system. As an illustration, consider a simple example in which the transition probabilities R_{ij} between states 1 and 2 are both ½. The solutions for P_i (i=1,2) will be:

$$P_1(t) = \frac{1}{2} + \frac{P_1(0) - P_2(0)}{2}e^{-2t}$$

$$P_2(t) = \frac{1}{2} + \frac{P_2(0) - P_1(0)}{2}e^{-2t} \tag{4}$$

We can see from the above that with increasing time, the second term, containing the initial state information, approaches zero and one is left with the equilibrium distribution $P_1(t_\infty) = P_1(t_\infty) = \frac{1}{2}$. Thus, the equilibrium distribution is the final result, without regard to the initial state. Determinism is broken.

Let us now examine how irreversibility 'sneaks in' between the time-reversible evolution of the basis-independent density operator ρ (obeying the Liouville equation) and that of the basis-dependent density matrix $\tilde{\rho}$ (obeying master equations employing transition rates between the occupied states). Pauli's "random phase assumption" [6] is behind this crucial distinction between the density operator and the density matrix, which for the diagonal case, must be physically arrived at through a non-unitary transition (if it is not to be brought in as an *ad hoc* assumption).

First, recall that the Von Neumann entropy S_{VN} is defined in terms of the density operator in a basis-independent way as:

$$S_{VN} = -Tr(\rho ln\rho) \tag{5}$$

Now, in order to employ the back-and-forth 'detailed balance' between states needed for master equations, one must work within a particular basis corresponding to transitions between the relevant states. So rather than work with the density operator, one must use a diagonal density matrix:

$$\tilde{\rho} = \sum_i P_i \, |i\rangle\langle i| \tag{6}$$

where P_i is the probability that the system is in state $|i\rangle$. In that basis, (5) becomes

$$S = -\sum_i (P_i ln P_i) \tag{7}$$

This form (the Shannon entropy) is well-defined only for the basis in which ρ is diagonal, and that is the "smuggling in" of irreversibility. In effect, it assumes that the system has been projected into that basis, a non-unitary process.

3. The Transactional Interpretation

In view of the above considerations regarding the "Process 1" measurement transition, we explore herein the view that the puzzle of the "initial probability assumption" referred to by Sklar is traceable to the measurement transition. The Transactional Interpretation (TI) provides an ontological basis for the measurement transition, lacking in Von Neumann's formulation, and as such is in a position to solve this 'central puzzle.'

3.1. Background

Before turning to the specifics of TI, it is worth noting that Einstein himself posited a fundamental quantum irreversibility associated with the particle-like aspect of light. Since it is the latter that accounts for the measurement transition and accompanying irreversibility in the TI model, let us revisit his comments on this point:

> In the kinetic theory of molecules, for every process in which only a few elementary particles participate (e.g., molecular collisions), the inverse process also exists. But that is not the case for the elementary processes of radiation. According to our prevailing theory, an oscillating ion generates a spherical wave that propagates outwards. The inverse process does not exist as an elementary process. A converging spherical wave is mathematically possible, to be sure; but to approach its realization requires a vast number of emitting entities. *The elementary process of emission is not invertible*. In this, I believe, our oscillation theory does not hit the mark. Newton's emission theory of light seems to contain more truth with respect to this point than the oscillation theory since, first of all, the energy given to a light particle is not scattered over infinite space, but remains available for an elementary process of absorption. [7]; emphasis added]

Einstein recognizes that, for a single quantum, all the energy represented by an isotropically propagating wave ends up being delivered to only a single absorbing system; thus the process acquires a final anisotropy (i.e., a directional momentum) not present initially. Recalling our discussion about the transforming of a density operator (which could be a pure state) to a diagonal density matrix (which is a mixed state), we see that the final anisotropy is the realization of one of the momentum components of the mixed state—i.e., collapse. The latter is a feature of the particle-like aspect of light, and that is what makes the process non-invertible. (This microscopic origin of irreversibility was also pointed out by Doyle [8].) As we will see, TI acknowledges both a wavelike and particlelike aspect to light; however it is the latter that brings about the irreversibility, just as Einstein noted.

The Transactional Interpretation was first proposed by Cramer [9] based on the Wheeler-Feynman direct-action theory of classical fields [10,11]. Its recent development by the present author [12-17] is based on the fully relativistic direct-action quantum theory of Davies [18,19]. In view of this relativistic development, the model is now referred to as the Relativistic Transactional Interpretation (RTI). It should perhaps be noted at the outset that TI is not considered a 'mainstream' interpretation, since its underlying model of fields—the direct-action theory—has historically been viewed with various degrees of skepticism. Nevertheless, despite the counterintuitive nature of the model, which includes advanced solution to the field equations, there is nothing technically wrong with it. (See [17] for why Feynman's abandonment of his theory was unnecessary.) Moreover, no less a luminary than John A. Wheeler was recently attempting to resurrect the direct-action theory in the service of progress toward a theory of quantum gravity. It's worth quoting from that paper here, in order to allay any concerns about the basic soundness of the model:

> [WF] swept the electromagnetic field from between the charged particles and replaced it with "half-retarded, half advanced direct interaction" between particle and particle. It was the high point of this work to show that the standard and well-tested force of reaction of radiation on an accelerated charge is accounted for as the sum of the direct actions on that charge by all the charges of any distant complete absorber. Such a formulation enforces global physical laws, and results in a quantitatively correct description of radiative phenomena, without assigning stress-energy to the electromagnetic field. ([20], p. 427)

Thus, there is no technical reason to eliminate the direct-action approach, and every reason to reconsider it in connection with such longstanding problems as the basis of the Second Law.

3.2 Measurement in TI

An overview of TI is provided in [16] ; we will not repeat that background information in this section, but will focus here on the TI account of the measurement transition. For present purposes it is sufficient to recall that according to TI, the usual quantum state or 'ket' $|\Psi\rangle$ is referred to as an 'offer wave' (OW), or sometimes simply 'offer' for short. The unfamiliar and counter-intuitive aspect of the direct action theory is inclusion of the solution to the complex conjugate (advanced) Schrodinger equation; this is the dual or 'brac,' $\langle X_i|$, describing the response of one or more absorbers X_i to the component of the offer received by them. The advanced responses of absorbers are termed 'confirmation waves' (CW).[2] Specifically, an absorber X_k will receive an offer wave component $\langle X_k|\Psi\rangle|X_k\rangle$ and will respond with a matching adjoint confirmation $\langle\Psi|\, X_k\rangle\langle X_k|$. The product of the offer/confirmation exchange is a weighted projection operator, $\langle X_k|\Psi\rangle\, \langle\Psi|\, X_k\rangle\; |X_k\rangle\langle X_k| = |\langle X_k|\Psi\rangle|^2|X_k\rangle\langle X_k|$. Clearly, the weight is the Born Rule, and this is how TI provides a physical origin for this formerly *ad hoc* rule. When one takes into account the responses of all the other absorbers $\{ X_i \}$, what we have is the von Neumann measurement transition from a pure state to a mixed state $\tilde{\rho}$:

$$|\Psi\rangle \;\rightarrow\; \tilde{\rho} = \sum_i |\langle\Psi|X_i\rangle|^2|X_i\rangle\langle X_i| \qquad (8)$$

In the absence of absorber response, the emitted offer wave (OW), $|\Psi\rangle$, is described by the unitary evolution of the time-dependent Schrodinger equation. Equivalently, in terms of a density operator $\rho = |\Psi\rangle\langle\Psi|$, its evolution can be described by its commutation with the Hamiltonian, as in (2).[3] However, once the OW $|\Psi\rangle$ prompts response(s) $\langle X_i|$ from one or more absorbers $\{X_i\}$, the linearity of this deterministic propagation is broken, and we get the non-unitary transformation (8).

Thus, according to TI, absorber response is what triggers the measurement transition. (Precise quantitative, though indeterministic, conditions for this response are discussed in [14].) It is the

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response of absorbers that transforms the density operator ρ, not committed to any basis, to the "density matrix" $\tilde{\rho}$, now *physically committed to the basis defined by the absorber response*, as shown in (8). And in fact it is here that the "probability assumption" enters in a physically justified manner, since the system is now physically described by a set of random variables (the possible outcomes) subject to a Kolmogorov (classical) probability space.

The second step in the measurement transition is non-unitary collapse to one of the outcomes $|X_k\rangle\langle X_k|$ from the set of possible outcomes $\{i\}$ represented by the weighted projection operators $|\langle\Psi|X_i\rangle|^2|X_i\rangle\langle X_i|$ in the density matrix $\tilde{\rho}$ above. This can be understood as a generalized form of spontaneous symmetry breaking, a *weighted* symmetry breaking: i.e., actualization of one of a set of possible states where in general the latter may not be equally probable. This is where Einstein's particle-like aspect enters. For example, an emitted isotropic (spherical) electromagnetic offer wave is ultimately absorbed by only one of the many possible absorbers that responded to it with CWs. The transferred quantum of electromagnetic energy acquires an anisotropy: a single directional momentum corresponding to the orientation of the 'winning' absorber. All the other possible momentum directions are not realized. The anisotropic directedness of the actualized spatial momentum component corresponds to the particle-like aspect or photon.

Thus, the measurement transition defines the point at which the unitary evolution ceases to apply, and the nonunitary 'master equation,' with probabilistic transition rates, enters as the correct physical description. Master equations necessarily work with well-defined probability spaces, with respect to particular bases corresponding to physically realized state transitions between emitters and absorbers in the studied thermodynamic system (e.g., a box of gas). Master equations cannot therefore apply to a system in the absence of absorber response, whose description is a ket $|\Psi\rangle$ or density operator ρ not committed to any particular basis (i.e., physical context). The apparent contradiction between the deterministic time-evolution of the density operator (2) and the indeterministic, probabilistic evolution respresented by master equations can be thereby resolved; the probabilistic description characterizing the transition from unitary to non-unitary evolution corresponds to the physical measurement transition triggered by absorber confirmations, which take the density operator ρ to the relevant density matrix , $\tilde{\rho}$.

In view of the above, it is apparent that a physically real measurement transition naturally fixes the basis (i.e. provides the context justifying (6)) and thus yields the well-defined probabilistic behavior instantiating Boltzmann's *Stosszahlansatz*. If interacting systems are engaging in continual emission/absorption events constituting 'Process 1,' these project the systems into specific quantum states, destroying the quantum coherence represented by the Von Neumann entropy (5). Between confirming interactions (those being inelastic as opposed to elastic), component systems may be described by deterministic (unitary) evolution; but with every such interaction, that evolution is randomized through the underlying quantum non-unitarity.

Thus, it is important to take into account that interacting atoms and molecules undergo state changes not simply due to elastic collisions (as in the usual classical picture), but due to inelastic interactions; i.e., absorption and re-emission of thermal photons. According to RTI, these are all transactions, accompanied by non-unitary collapses, and are therefore truly random processes. The thermodynamical implications are clear: in a closed interacting system described by the Second Law (such as a box of gas with internal energy U), the component systems are continually undergoing internal state changes, chiefly thermal excitations and de-excitations. Each such process is inherently random according to RTI. That is, the statistical description that Boltzmann derived based on his *Stosszahlansatz* is based on a real physical process.

4. The Relativistic Level: Further Roots of the Arrow of Time

At the deeper, relativistic level of RTI, the generation of absorber response (i.e. a confirmation) is itself a stochastic process described (in part) by coupling amplitudes between fields. For example, the random Poissonian probabilistic description of the decay of an atomic electron's excited state is understood in the transactional picture as reflecting a real ontological indeterminacy in the generation of both an offer and confirmation for the photon emitted. Details of the transactional model of the inherently probabilistic nature of atomic decays and excitations are given in [14]. The same basic picture applies to other kinds of decays (i.e. of nuclei or composite quanta), since all such decays occur due to coupling among the relevant fields.

Considering the relativistic level also allows us to identify a basic source of temporal asymmetry corresponding to that pointed out by Einstein above. In the direct-action theory, the state of the quantum electromagnetic field resulting from absorber response to the basic time-symmetric propagation from an emitter is a Fock state (or superposition of Fock states)[14]. These correspond to 'real photons; they are quantized, positive-energy excitations of the field (this applies to antiparticles as well; see [17]). Such states can be represented by the action of creation operators $\hat{a}^{\dagger}$ on the vacuum state of the field. E.g., a single photon state of energy k is given by:

$$|k\rangle = \hat{a}^{\dagger}{}_{k}|0\rangle$$

Meanwhile, the confirming response, a 'brac' or dual ket $\langle k|$, can be represented as the annihilation operator $\hat{a}_k$ acting to the left on the dual vacuum, i.e.:

$$\langle k| = \langle 0|\hat{a}_k$$

The relevant point is that there is an intrinsic temporal asymmetry here: *a field excitation must be created before it can be destroyed* (or, equivalently, responded to by an absorbing system). This seemingly obvious and mundane fact is actually a crucial ingredient in the origin of the temporal arrow: any emission must precede the corresponding absorption. An emission event therefore must always be in the past relative to its matching absorption event. This is simply because one cannot destroy something that does not exist: a thing must first exist in order to be destroyed. The basic relativistic field actions of creation and annihilation therefore presuppose temporal asymmetry. This asymmetry is reflected in the distinctly different actions of the creation and annihilation operators on the vacuum state:

$$\hat{a}^{\dagger}{}_{k}|0\rangle = |k\rangle; \text{ whereas } a_k|0\rangle = 0.$$

Thus, if one tries to annihilate something that doesn't exist, one gets no state at all—not even the vacuum state.

The above is why the indeterministic collapse to one out of many possible outcomes also yields a temporal directionality—i.e., an arrow of time. The chosen outcome always corresponds to delivery of a quantum of energy (and, in general, other conserved quantities such as momentum, angular momentum, etc). Energy is the generator of temporal displacement, and since a quantum must be created before it is destroyed, the energy transfer always defines a temporal orientation *from* the emitter (locus of creation) *to* the absorber (locus of annihilation). Moreover, the delivered energy is always positive, corresponding to a positive temporal increment [17].[4]

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[4] The direct action theory is subject to a choice of boundary conditions for the superposition of the time-symmetric fields from emitters and absorbers leading to the free field component needed for real (on-shell) energy propagation. The choice discussed herein corresponds to the choice of Feynman propagation. It is possible to choose Dyson rather than Feynman propagation, but the resulting world is indistinguishable from our own; the definition of 'negative' vs 'positive' energy is just a convention in that context. For further discussion of this issue, in terms of Gamow vectors and resulting microscopic proper time asymmetry, see [21].

5. Conclusion

It has been shown that if the non-unitary measurement transition of Von Neumann is a physically real component of quantum theory, then the representation of the system(s) under study by diagonal density matrices, subject to master equation description, is physically justified.

According to the TI account of measurement, a quantum system undergoes a real, physical non-unitary state transition based on absorber response. Thus the system's probabilistic description is justified. This can be understood as the origin of the 'initial probability assumption' referred to as puzzling by Sklar. However, in this model, it ceases to be an assumption and can be seen as describing a physical feature of Nature. In addition, the relativistic level of TI (referred to as RTI) provides a basis for the directionality of the irreversibility inherent in the measurement transition, thereby establishing an arrow of time consistent with the Second Law. In this respect, the arrow of time is not *explained by* entropy increase; rather, it is a crucial component of the *explanation for* the increase in entropy toward the future.

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