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Abstract. We discuss the structure and main features of the nonlinear evolution equation proposed by this author as the fundamental dynamical law within the framework of Quantum Thermodynamics. The nonlinear equation generates a dynamical group providing a unique deterministic description of irreversible, conservative relaxation towards equilibrium from any non-equilibrium state, and satisfies a very restrictive stability requirement equivalent to Hatsopoulos-Keenan statement of the second law of thermodynamics. Here, we emphasize its mathematical structure and its applicability also within other contexts, such as Classical and Quantum Statistical Mechanics, and Information Theory.

Keywords: Nonlinear Dynamics Dynamics; Irreversibility; Entropy; Information Theory; Quantum Thermodynamics
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INTRODUCTION

The problem of understanding entropy and irreversibility has been tackled by a large number of preeminent scientists during the past century. Schools of thought have formed and flourished around different perspectives of the problem. But a definitive solution has yet to be found.

We address a mathematical problem very relevant to the question of nonequilibrium and irreversibility, namely, that of "designing" a general evolution equation capable of describing irreversible but conservative relaxation towards equilibrium. Our objective is to present an interesting mathematical solution to this "design" problem, namely, a new nonlinear evolution equation that satisfies a set of very stringent, relevant requirements [1].

We first define four essentially different contexts within which the new equation is clearly relevant, with entirely different interpretations: Classical Statistical Mechanics (CSM), Classical Information Theory (CIT), Quantum Statistical Mechanics (QSM), Quantum Thermodynamics (QT). Then, we list the "design specifications" that we intend to impose on the desired evolution equation. We review some useful well-known mathematics involving Gram determinants and, finally, present our nonlinear evolution equation which meets the stringent design specifications.

The discussion here is purposely devoided of our school's quite unorthodox perspective, views and hypotheses on the physical meaning of entropy and irreversibility. This is not only due to obvious space limitations, but mainly because we feel that the proposed nonlinear equation constitutes an important mathematical-physics advance in itself not only in the Quantum Thermodynamics contexts for which it was originally designed and developed [2–7], but also in other contexts, such as CSM, CIT, QSM, as well as possibly in Quantum Information, Biology, Sociology and Economics.

FRAMEWORK A: CLASSICAL STATISTICAL MECHANICS

Let Ω be a phase space, and $\mathscr{L}$ the set of real, square-integrable functions $A, B, \ldots$ on Ω, equipped with the inner product $(\cdot|\cdot)$ defined by

$$(A|B) = \text{Tr}(AB) = \int_\Omega AB \, d\Omega \tag{1}$$

where $\text{Tr}(\cdot)$ in this framework denotes $\int_\Omega \cdot \, d\Omega$. We denote by $\mathscr{P}$ the subset of all nonnegative-definite, normalized functions (distributions) ρ in $\mathscr{L}$, i.e.,

$$\mathscr{P} = \left\{ \rho \text{ in } \mathscr{L} \,|\, \rho \geq 0, \text{Tr}(\rho) = \int_\Omega \rho \, d\Omega = 1 \right\} \tag{2}$$

We will then consider a set $\{H, N_1, \ldots, N_r\}$ of functions in $\mathscr{L}$.

In Classical Statistical Mechanics, ρ is the Gibbs density-of-phase distribution function which represents the index of statistics from a generally heterogeneous ensemble of identical systems (with associated phase space Ω) distributed over a range of possible classical mechanical states (the support of ρ). H is the Hamiltonian function, and N_i the number-of-particle function for particles of type i.

FRAMEWORK B: CLASSICAL INFORMATION THEORY

Let $\mathscr{L}$ be the set of all $n \times n$ real, diagonal matrixes $A = \mathrm{diag}(a_j)$, $B = \mathrm{diag}(b_j)$, $\ldots$ ($n \leq \infty$), equipped with the inner product $(\cdot|\cdot)$ defined by

$$(A|B) = \mathrm{Tr}(AB) = \sum_{j=1}^{n} a_j b_j \tag{3}$$

We denote by $\mathscr{P}$ the subset of all nonnegative-definite, unit-trace matrixes ρ in $\mathscr{L}$, i.e.,

$$\mathscr{P} = \left\{ \rho = \mathrm{diag}(p_j) \,|\, p_j \geq 0,\ \mathrm{Tr}(\rho) = \sum_{j=1}^{n} p_j = 1 \right\} \tag{4}$$

Later we consider a set $\{H, N_1, \ldots, N_r\}$ of diagonal matrixes $H = \mathrm{diag}(e_j)$, $N_1 = \mathrm{diag}(n_{1j})$, $\ldots$, $N_r = \mathrm{diag}(n_{rj})$ in $\mathscr{L}$.

In Information Theory [8], $\rho = \mathrm{diag}(p_j)$ represents the probability assignment to a set of n events, p_j being the probability of occurrence of the j-th event. H, N_1, $\ldots$, N_r are characteristic features of the events in the set, taking on the values $e_j, n_{1j}, \ldots, n_{rj}$, respectively, for the j-th event.

FRAMEWORK C: QUANTUM STATISTICAL MECHANICS

Let $\mathscr{H}$ be a Hilbert space (dim $\mathscr{H} \leq \infty$), and $\mathscr{L}$ the set of all linear operators A, B, $\ldots$ on $\mathscr{H}$, equipped with the real inner product $(\cdot|\cdot)$ defined by

$$(A|B) = \mathrm{Tr}\left(A^{\dagger}B + B^{\dagger}A\right)/2 \tag{5}$$

where $A^{\dagger}$ denotes the adjoint of operator A and $\mathrm{Tr}(\cdot)$ the trace functional. We denote by $\mathscr{P}$ the set of all self-adjoint, nonnegative-definite, unit-trace operators ρ in $\mathscr{L}$, i.e.,

$$\mathscr{P} = \left\{ \rho \text{ in } \mathscr{L} \,|\, \rho^{\dagger} = \rho, \rho \geq 0, \mathrm{Tr}\rho = 1 \right\} \tag{6}$$

We will then consider a set $\{H, N_1, \ldots, N_r\}$ of self-adjoint operators in $\mathscr{L}$, where each N_i commutes with H, i.e., is such that $HN_i = N_iH$, for $i = 1, \ldots, r$.

In Quantum Statistical Mechanics, ρ is the von Neumann statistical or density operator which represents the index of statistics from a generally heterogeneous ensemble of identical systems (same Hilbert space $\mathscr{H}$ and operators $\{H, N_1, \ldots, N_r\}$) distributed over a range of generally different quantum mechanical states. If each individual member of the ensemble is isolated and uncorrelated from the rest of the universe, its state is described according to Quantum Mechanics by an idempotent density operator ($\rho^2 = \rho = P_{|\psi\rangle} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$), i.e., a projection operator onto the span of some vector $|\psi\rangle$ in $\mathscr{H}$. If the ensemble is heterogeneous, its individual member systems may be in different states, $P_{|\psi_1\rangle}, P_{|\psi_2\rangle}$, and so on.

H is the Hamiltonian operator, and operator N_i, for $i = 1, \ldots, r$, is the number operator for particles of type i in the system (if the system has a fixed number n_i of particles of type i, then $N_i = n_i I$, where I is the identity operator on $\mathscr{H}$).

FRAMEWORK D: QUANTUM THERMODYNAMICS

In our formulation of Quantum Thermodynamics [2–6], the mathematical framework is the same as that just summarized for QSM, but the fundamental difference is in the physical meaning of the density operator. Indeed, QT assumes that the true individual quantum state of a system isolated and uncorrelated from the rest of the universe is represented by a density operator ρ which are not necessarily idempotent. Over the set of idempotent ρ's, QT coincides with Quantum Mechanics, but it differs fundamentally from it because it assumes a broader set of possible states, corresponding to the set of non-idempotent ρ's. This way, the functional $S(\rho)$ (defined in the next section) describes in QT an intrinsic (non-statistical) fundamental state property of the individual system. This is very different from the meaning that the von Neumann functional $S(\rho)$ has in QSM, where it measures the degree of heterogeneity of the ensemble whose statistics are represented by ρ.

MEAN VALUE FUNCTIONALS AND S-FUNCTIONAL

From here on, our notation allows us to treat at once the four contexts just defined. For reasons to become apparent below, the elements $H, N_1, \ldots, N_r$ introduced in either context, will be called the generators of the motion (MG). We assume that such sets always contain at least element H, that we call the Hamiltonian MG.

For each MG, we then define a mean value functional on $\mathscr{P}$ as follows

$$m(\rho;H) = \mathrm{Tr}\rho H = (\sqrt{\rho}|\sqrt{\rho}H) \quad, \qquad m(\rho;N_i) = \mathrm{Tr}\rho N_i = (\sqrt{\rho}|\sqrt{\rho}N_i) \tag{7}$$

Moreover, we define the S-functional [9] on $\mathscr{P}$ as

$$S(\rho) = -k\mathrm{Tr}(\rho\ln\rho) = -k(\sqrt{\rho}|\sqrt{\rho}\ln\rho) \tag{8}$$

Depending on the context, the S-functional represents the statistical uncertainty as to the actual classical or quantum state of a system, the information carried by the occurrence of one of the possible events (or the degree of uncertainty as to which will be the next event), or the thermodynamic entropy.

For each given set of values $\langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle$, in the range of the mean value functionals (Eqs. 7) corresponding to the GM's, we consider the subset of all elements ρ in $\mathscr{P}$ that share the given mean values, i.e.,

$$\mathscr{P}_{\{\langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle\}} = \{\rho \text{ in } \mathscr{P} \,|\, m(\rho;H) = \langle H \rangle, m(\rho;N_i) = \langle N_i \rangle \text{ for } i = 1, \ldots, r\} \tag{9}$$

On each such subset, i.e., for fixed mean values $\langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle$ of the generators of the motion, the S-functional (Eq. 8) achieves a unique maximum at the point

$$\rho = e^{-\alpha}\exp\left(-\beta H + \sum_{i=1}^r v_i N_i\right) \quad \text{where} \quad \alpha = \ln\mathrm{Tr}\left[\exp\left(-\beta H + \sum_{i=1}^r v_i N_i\right)\right] \tag{10}$$

and, of course, $\beta = \beta(\langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle)$ and $v_i = v_i(\langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle)$. It is noteworthy that the maximum-S points satisfy the condition

$$\sqrt{\rho}\ln\rho = -a\sqrt{\rho} - b\sqrt{\rho}H + \sum_{i=1}^r c_i\sqrt{\rho}N_i \tag{11}$$

for some real numbers a, b and c_i, $i = 1, \ldots, r$. In words, the maximum-S element ρ is such that $\sqrt{\rho}\ln\rho$ lies in the linear manifold generated by elements $\sqrt{\rho}, \sqrt{\rho}H, \sqrt{\rho}N_1, \ldots, N_r$. Condition 11 is satisfied not only by the maximum-S elements given by Eq. 10, but also by the elements given by

$$\rho = e^{-a}B\exp\left(-bH + \sum_{i=1}^r c_i N_i\right)B \quad \text{where} \quad a = \ln\mathrm{Tr}\left[B\exp\left(-bH + \sum_{i=1}^r c_i N_i\right)B\right] \tag{12}$$

where $b = b(B; \langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle)$, $c_i = c_i(B; \langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle)$ and B is any idempotent element in $\mathscr{L}$ (i.e., $B^2 = B$). Clearly, Eq. 12 reduces to Eq. 10 iff $B = I$ (I = constant function equal to 1 on the whole Ω in CSM; $I = \mathrm{diag}(1)$ in CIT; I = identity operator on $\mathscr{H}$ in QSM and QT).

DYNAMICAL LAW DESIGN SPECIFICATIONS

Our scope is to design a function $F(\cdot)$ such that every solution $\rho(t)$ of the autonomous differential equation

$$\frac{d}{dt}\rho(t) = F(\rho(t)) \tag{13}$$

with $\rho(0)$ anywhere in $\mathscr{P}$ satisfies the following conditions for all t's, $-\infty < t < \infty$:

(i) $\rho(t)$ lies entirely in $\mathscr{P}$ (no forward nor backward escape times);

(ii) $m(\rho(t);H) = m(\rho(0);H)$, and $m(\rho(t);N_1) = m(\rho(0);N_i)$ for $i = 1, \ldots, r$;

(iii) $S(\rho(t+u)) \geq S(\rho(t))$ for all $u > 0$;

(iv) within each subset $\mathscr{P}_{\{\langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle\}}$, the maximum-$S$ element given by Eq. 10) is the only equilibrium solution that is stable according to Lyapunov [9]; all other equilibrium elements must not be stable.

Notice that requirement (iv) is most restrictive. For example, within QSM, it rules out the von Neumann evolution equation ($F(\rho) = -i(H\rho - \rho H)/\hbar$) because all the stationary density matrices (ρ such that $H\rho = \rho H$) are stable according to Lyapunov and, in general, there are many more than a single one within each set $\mathscr{P}_{\{\langle H \rangle, \langle N_1 \rangle, \ldots, \langle N_r \rangle\}}$.

SOME NECESSARY MATHEMATICAL BACKGROUND

Given a subset of elements $A, B, \ldots, Z$ in $\mathscr{L}$, we denote by $M(A, B, \ldots, Z)$ the Gram matrix

$$
\begin{bmatrix}
(A|A) & (A|B) & \ldots & (A|Z) \\
(B|A) & (B|B) & \ldots & (B|Z) \\
\vdots & \vdots & \ddots & \vdots \\
(Z|A) & (Z|B) & \ldots & (Z|Z)
\end{bmatrix}
\tag{14}
$$

where $(\cdot|\cdot)$ is the real symmetric inner product defined on $\mathscr{L}$. We denote by $G(A, B, \ldots, Z)$ the Gram determinant of $A, B, \ldots, Z$ with respect to inner product $(\cdot|\cdot)$, i.e., $G(A, B, \ldots, Z) = \det[M(A, B, \ldots, Z)]$. Matrix $M(A, B, \ldots, Z)$ is nonnegative definite and $G(A, B, \ldots, Z)$ is nonnegative. Elements $A, B, \ldots, Z$ are linearly independent (LI) iff their Gram determinant $G(A, B, \ldots, Z)$ is nonzero and, hence, strictly positive.

Given a subset of elements $A, B, \ldots, Z$ in $\mathscr{L}$, we denote by $L(A, B, \ldots, Z)$ the linear manifold spanned by all linear combinations with real coefficients of the elements $A, B, \ldots, Z$. With respect to the inner product $(\cdot|\cdot)$ defined on $\mathscr{L}$, we denote the projection of a given element V in $\mathscr{L}$ onto a linear manifold L by the symbol $(V)_L$. $(V)_L$ is the unique element in L such that $((V)_L|X) = (V|X)$ for all X in L.

The theory of Gram determinants, very seldom used in the physics literature, offers a useful explicit way of writing the projection $(V)_L$ of V onto a given linear manifold L. Let the given linear manifold be $L = L(A, B, \ldots, Z)$, where elements $A, B, \ldots, Z$ need not be LI. Select any subset of LI elements $E_1, E_2, \ldots, E_m$ spanning L, i.e., such that $G(E_1, E_2, \ldots, E_m) > 0$ and $L(E_1, E_2, \ldots, E_m) = L$. By the definition of $(V)_L$, $((V)_L|E_j) = (V|E_j)$ for every $j = 1, 2, \ldots, m$, and $(V)_L = \sum_{i=1}^{m} v_i E_i$, where v_i are real scalars. Thus,

$$
\sum_{i=1}^{m} v_i (E_i|E_j) = (V|E_j) \text{ for } j = 1, 2, \ldots, m
\tag{15}
$$

Because $(E_i|E_j) = [M(E_1, E_2, \ldots, E_m)]_{ij}$ and the elements $E_1, E_2, \ldots, E_m$ are LI, Eqs. 15 are LI and can be solved for the v_i's to yield

$$
v_i = \sum_{i=1}^{m} (V|E_j)[M(E_1, E_2, \ldots, E_m)^{-1}]_{ji} \quad \text{for } i = i = 1, 2, \ldots, m
\tag{16}
$$

and, therefore,

$$
(V)_L = \sum_{i=1}^{m} \sum_{j=1}^{m} (V|E_j)[M(E_1, E_2, \ldots, E_m)^{-1}]_{ji} E_i
\tag{17}
$$

Alternatively, Cramer's rule yields the equivalent, more elegant expression

$$
(V)_L = -\frac{1}{G(E_1, E_2, \ldots, E_m)} \det
\begin{bmatrix}
0 & E_1 & E_2 & \ldots & E_m \\
(E_1|V) & (E_1|E_1) & (E_1|E_2) & \ldots & (E_1|E_m) \\
(E_2|V) & (E_2|E_1) & (E_2|E_2) & \ldots & (E_2|E_m) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
(E_m|V) & (E_m|E_1) & (E_m|E_2) & \ldots & (E_m|E_m)
\end{bmatrix}
\tag{18}
$$

Below, for any given element ρ in the set $\mathscr{P}$, we will need to consider the projection of $\sqrt{\rho} \ln \rho$ onto the linear manifold $L(\sqrt{\rho}, \sqrt{\rho}H, \sqrt{\rho}N_1, \ldots, \sqrt{\rho}N_r)$ where $\sqrt{\rho}, \sqrt{\rho}H, \sqrt{\rho}N_1, \ldots, \sqrt{\rho}N_r$ are not necessarily LI. Using Eq. 18 and Definitions 1, 3 and 5 of the inner product $(\cdot|\cdot)$, we find

$$
(\sqrt{\rho} \ln \rho)_{L(\sqrt{\rho}, \sqrt{\rho}H, \sqrt{\rho}N_1, \ldots, \sqrt{\rho}N_r)} = -\frac{1}{G\left(\sqrt{\rho}R_0, \sqrt{\rho}R_1, \ldots \sqrt{\rho}R_z\right)} \times
\tag{19}
$$

$$
\times \det
\begin{bmatrix}
0 & \sqrt{\rho}R_0 & \sqrt{\rho}R_1 & \ldots & \sqrt{\rho}R_z \\
\mathrm{Tr}\rho \ln \rho & \mathrm{Tr}\rho R_0^2 & \frac{1}{2}\mathrm{Tr}\rho\{R_0, R_1\} & \ldots & \frac{1}{2}\mathrm{Tr}\rho\{R_0, R_z\} \\
\mathrm{Tr}\rho R_1 \ln \rho & \frac{1}{2}\mathrm{Tr}\rho\{R_1, R_0\} & \mathrm{Tr}\rho R_1 & \ldots & \frac{1}{2}\mathrm{Tr}\rho\{R_1, R_z\} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\mathrm{Tr}\rho R_z \ln \rho & \frac{1}{2}\mathrm{Tr}\rho\{R_z, R_0\} & \frac{1}{2}\mathrm{Tr}\rho\{R_z, R_1\} & \ldots & \mathrm{Tr}\rho R_z^2
\end{bmatrix}
\tag{20}
$$

where $\{A, B\} = AB + BA$, and $R_0, R_1, \ldots, R_z$ are a subset of elements in $\mathscr{L}$ such that $L(\sqrt{\rho}R_0, \sqrt{\rho}R_1, \ldots, \sqrt{\rho}R_z) = L(\sqrt{\rho}, \sqrt{\rho}H, \sqrt{\rho}N_1, \ldots, \sqrt{\rho}N_r)$ and $G(\sqrt{\rho}R_0, \sqrt{\rho}R_1, \ldots, \sqrt{\rho}R_z) > 0$.

STEPEEST-S-ASCENT NONLINEAR EVOLUTION EQUATION

With the above background, the nonlinear evolution equation proposed by the author [3–6, 10] to meet our design specifications takes the compact form:

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H,\rho] - \frac{1}{2\tau}\left(\sqrt{\rho}D(\rho) + D^{\dagger}(\rho)\sqrt{\rho}\right) \tag{21}$$

$$D(\rho) = \sqrt{\rho}\ln\rho - (\sqrt{\rho}\ln\rho)_{L\left(\sqrt{\rho},\sqrt{\rho}H,\sqrt{\rho}N_1,\ldots,\sqrt{\rho}N_r\right)} \tag{22}$$

where $[H,\rho] = H\rho - \rho H$ (= 0 within CSM and CIT), $\hbar$ is the reduced Planck constant (playing a role only within QSM and QT), τ is a characteristic time constant, $H, N_1, \ldots, N_r$ are fixed GM's.

Notice that $D(\rho(t))$ is orthogonal to the linear manifold spanned by $\sqrt{\rho}(t), \sqrt{\rho}(t)H, \sqrt{\rho}(t)N_1, \ldots, \sqrt{\rho}(t)N_r$ and the term $i[H,\rho]$ is orthogonal to $\sqrt{\rho}D(\rho) + D^{\dagger}(\rho)\sqrt{\rho}$.

Within QT, if the isolated and uncorrelated system AB is composed of subsystems A (Alice) and B (Bob) that are either interacting ($H = H_A \otimes I_B + I_A \otimes H_B + V_{AB}$) or correlated ($S \neq S_A \otimes I_B + I_A \otimes S_B$, where $S = -k_B(P_{\text{Ran}\rho})\ln\rho$), or both, the proposed equation takes the form [6, 10] (we assume for simplicity that A and B have no non-Hamiltonian GM's):

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho] + \frac{1}{2k_B\tau_A}\left(\sqrt{\rho_A}D_A + D_A^{\dagger}\sqrt{\rho_A}\right) \otimes \rho_B + \frac{1}{2k_B\tau_B}\rho_B \otimes \left(\sqrt{\rho_B}D_B + D_B^{\dagger}\sqrt{\rho_B}\right) \tag{23}$$

$$
\begin{aligned}
D_A &= \sqrt{\rho_A}(S)^A - [\sqrt{\rho_A}(S)^A]_{L\{\sqrt{\rho_A},\sqrt{\rho_A}(H)^A\}} & D_B &= \sqrt{\rho_B}(S)^B - [\sqrt{\rho_B}(S)^B]_{L\{\sqrt{\rho_B},\sqrt{\rho_B}(H)^B\}} \\
(H)^A &= \text{Tr}_B[(I_A \otimes \rho_B)H] & (H)^B &= \text{Tr}_A[(\rho_A \otimes I_B)H] \\
(S)^A &= \text{Tr}_B[(I_A \otimes \rho_B)S] & (S)^B &= \text{Tr}_A[(\rho_A \otimes I_B)S]
\end{aligned} \tag{24}
$$

Despite the nonlinearity, the structure of the non-Hamiltonian terms in the equation prevents "no-signaling" violations.

All zero entropy states ($\rho^2 = \rho$), even if A and B are entangled, obey the Schroedinger equation $\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho]$, thus not contradicting any of the results of QM, although within QT, these solutions, including the stationary states of QM ($\rho^2 = \rho$, $\rho H = H\rho$) are very weakly unstable limit cycles or equilibrium states [11].

The proofs that this equations satisfy our design specification are in Refs. [5–7, 10, 12]. Several other intriguing features including Onsager's reciprocal relations are discussed in Refs. [11–13]. Eq. 23 generalizes Eq. 21 to composite systems consistently with the additional design specs required to avoid non-locality paradoxes [6, 10].

We believe that in view of its intriguing properties, this evolution equation constitutes an important mathematical "tool" for a variety of non-equilibrium relaxation problems, not only within our QT, but also within different contexts, such as CSM, CIT, and QSM, as discussed here, as well as Quantum Information, Biology, Sociology and Economics. Even in the Thermodynamics context, where different schools of thought notoriously have contrasting perspectives on the physical meaning of entropy and irreversibility, many important insights can nevertheless be extracted from the richness of structure and the well-behaved and self-consistent features of this relevant nonlinear dynamical equation.

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