Quantum Information Physics I

TR2021-996

Revised: March 25, 2022

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Abstract

Quantum physics, despite its intrinsic probabilistic nature, is formulated as time-reversible. We propose an entropy for quantum physics, which may conduce to the emergence of a time arrow. That entropy is a measure of randomness over the degrees of freedom of a quantum state and is quantified in quantum phase spaces. Its minimum is positive due to the uncertainty principle.

To study the relation of the entropy to physical phenomena, we classify the behaviors of quantum states according to their entropy evolution. We revisit transition probabilities and Fermi's golden rule to show their close relation to states with oscillating entropy. We study collisions of two particles in coherent states, and show that as they come closer to each other, their entanglement causes the total system's entropy to oscillate.

We conjecture an entropy law whereby the entropy never decreases, and speculate that entropy oscillations trigger the annihilations and the creations of particles.

CONTENTS

INTRODUCTION AND SUMMARY

Today's classical and quantum physics laws are time-reversible, and a time arrow emerges in physics only when a probabilistic behavior of ensembles of particles is considered. In contrast, no mechanism for a time arrow has been proposed for quantum physics even though it introduces probability as intrinsic to the description of even a single-particle system. The concept of entropy has been useful in classical physics but extending it to quantum mechanics (QM) has been challenging. For example, von Neumann entropy [22] requires the existence of classical statistics elements (mixed states) in order not to vanish, and consequently it must assign the entropy of 0 to one-particle states (pure states). Von Neumann entropy captures the randomness associated with not-knowing precisely the quantum state. Therefore, it is not possible to start with von Neumann entropy if one wants to assign an entropy that measures the randomness of a given pure quantum state. Wehrl entropy [23] is based on Husimi's [16] quasiprobability distribution, rooted in projecting states to an overcomplete basis representation of coherent states. Note that no two coherent states are orthogonal to each other. Therefore, Kolmogorov third axiom for a probability distribution, for events to be mutually exclusive, is not satisfied. Thus, probability properties such as for example, the monotonicity of probabilities and the complement rule, are not satisfied by Husimi's quasiprobability distribution. These limitations prevent Wehrl entropy from correctly counting the random values of the observables. Say we have just observed a particle in position space at $\mathbf{r}_0$. The state is then a peak at such a position. Projecting it onto coherent states, we will produce a non-zero value distribution for all possible position coordinates q in the phase space coordinate (q, p), where p is the momentum coordinate. Clearly, this is not the description of the random position observable $\mathbf{r}$ in QM. We require the quantum entropy to be invariant under special relativity transformations and under point-wise transformation of position coordinates (such as a spherical-polar coordinate change), and Wehrl entropy is not invariant under neither of these two transformations. Indeed Wehrl intent was to define an entropy for the classical phase space, an approximation to a quantum state, and not to construct a quantum entropy in quantum phase space. We point out that coherent states minimize the uncertainty principle [19], and as shown by Lieb [18] they also minimize Wehrl entropy. And as we show here, they also minimize our proposed entropy. We then argue that neither von Neumann entropy nor Wehrl entropy capture the exact amount of randomness associated with the observables of a pure quantum state.

In classical physics, Boltzmann entropy and Gibbs entropy and their respective H-theorems [14] are formulated in the classical phase space, reflecting the degrees of freedom (DOFs) of a system. In quantum physics the complete description of randomness of a particle state goes beyond the randomness of the DOFs of a state as illustrated by the uncertainty principle. Even though the momentum description of a state can be recovered by the position DOFs description of a state (via a Fourier transform), the randomness of the state is only captured in quantum phase space formed by position and momentum (or spatial frequency) projections of a quantum state. Note that there are internal DOFs, such as the spin orientation of a particle, which must be accounted for via their own phase space when quantifying total randomness.

As discussed by Wehrl [23], a quantum entropy is not an observable as there is no entropy operator, instead, entropy is a function associated with a state. We argue that the entropy in quantum physics must (i) account for all the DOFs of a state, (ii) be a quantification of randomness of the observables of such a state, and (iii) be invariant under the applicable transformations of the state. We propose an entropy defined in quantum phase spaces associated with the DOFs and that satisfies those conditions. We defined the quantum phases space to simultaneously be the space of all possible states projected in the position and a spatial frequency basis. It is applicable to both QM and Quantum Field Theory (QFT).

To analyze particles' evolution, we introduce a QCurve structure imposed on the evolutions of a quantum state. We partition the set of all the QCurves according to their entropies' behavior during an evolution.

An important set of QCurves is the one in which the entropy oscillates. This set includes the cases of transitions from one state to another with probabilities obtained from Fermi's golden rule. Fermi's golden rule is derived from a unitary evolution of a state. Consequently, for the hydrogen atom, in order to account for a transition from an excited state to the ground state with the emission of a photon, Fermi's golden rule assigns a coefficient to the ground state that increases with time while the coefficient assigned to the excited state decreases with time, but both states remain in a superposition. One can not conclude that the event of a photon creation and its emission either occur or not, unless an experiment is devised to observe the event, and the outcome may be that such transition does not occur.

In our study of the QCurves corresponding to the evolution of the hydrogen atom in an excited state, we show a close association between the entropy and Fermi's golden rule probabilities. The mathematical behavior of both is related as they both oscillate in tandem: first increasing and then decreasing. We then conjecture that there is an entropy law, universally applicable to particle physics, stating that the entropy never decreases in a physical scenario.

Then, such law acts as a trigger, "causing" the electron to jump to the ground state and emit a photon. In contrast to Fermi's golden rule probabilistic reasoning over the superposition of states, the entropy law guarantees that the jump does occur and a photon is emitted. Thus, the law provides a deterministic cause for that event. We examine this and other scenarios where such an entropy law may be applicable. From an information-theoretic point of view, such a law states that during the evolution of a physical scenario the information (the "inverse" of randomness) cannot be increased.

QUANTUM ENTROPY IN QUANTUM PHASE SPACES

The quantum entropy must account for both the coordinate and the internal (spin) DOFs, and we define the entropy in light of this requirement.

Coordinate-Entropy

We associate with a state $|\psi\rangle$ its projection onto the QM eigenstates of the operators $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$, i.e., $|\mathbf{r}\rangle$ and $|\mathbf{p}\rangle$. Either one projection, $\psi(\mathbf{r}) = \langle \mathbf{r}|\psi\rangle$ or $\phi(\mathbf{p}) = \langle \mathbf{p}|\psi\rangle$, is sufficient to recover the other one via a Fourier transform. We define the quantum coordinate phase space as the space of all possible states projected simultaneously in pairs $(\psi(\mathbf{r}),\ \phi(\mathbf{p}))$. The density operator associated with state $|\psi\rangle$ is $\rho = |\psi\rangle \langle\psi|$ and its time evolution according to a Hermitian Hamiltonian H is described by $\rho_t = \mathrm{e}^{-\mathrm{i}\frac{H}{\hbar}t}\rho \mathrm{e}^{\mathrm{i}\frac{H}{\hbar}t}$. Projecting the density operator into the quantum coordinate phase space we obtain the probability densities $\rho_{\mathrm{r}}(\mathbf{r},t) = \langle \mathbf{r}|\, \rho_t \,|\mathbf{r}\rangle = |\psi(\mathbf{r},t)|^2$ and $\rho_p(\mathbf{p},t) = \langle \mathbf{p}|\, \rho_t \,|\mathbf{p}\rangle = |\tilde{\phi}(\mathbf{p},t)|^2$. By considering a quantum coordinate phase space we will be able to capture the randomness of the coordinates of a particle as illustrated by the uncertainty principle. We argue that it is necessary to consider both projections in order to capture all the randomness of the observables, and in order to produce appropriate entropy invariance under applicable transformation (such as changes of position coordinates).

Our formulation of the entropy is clearly motivated by previous work, and we mention as examples, Gibbs [14], Shanon [21] and Jaynes [17]. Let the entropy associated only with the spatial coordinates be the differential entropy $\mathrm{S}_{\mathrm{r}} = -\int \rho_{\mathrm{r}}(\mathbf{r},t) \ln \rho_{\mathrm{r}}(\mathbf{r},t)\ \mathrm{d}^3\mathbf{r}$. Let $\mathbf{k} = \frac{1}{\hbar}\mathbf{p}$ be the spatial frequency, and $\rho_k(\mathbf{k},t) = \frac{1}{\hbar^3}\rho_p(\mathbf{p},t)$ the associated probability density, and $\mathrm{S}_{\mathrm{k}} = -\int \rho_{\mathrm{k}}(\mathbf{k},t) \ln \rho_{\mathrm{k}}(\mathbf{k},t)\ \mathrm{d}^3\mathbf{k}$. Then we define the entropy associated with the quantum coordinate phase space distributions as

$$\mathrm{S} = -\int \rho_{\mathrm{r}}(\mathbf{r},t)\rho_k(\mathbf{k},t)\ \ln\left(\rho_{\mathrm{r}}(\mathbf{r},t)\rho_k(\mathbf{k},t)\right)\ \mathrm{d}^3\mathbf{r}\ \mathrm{d}^3\mathbf{k} = \mathrm{S}_{\mathrm{r}} + \mathrm{S}_{\mathrm{k}}\,. \tag{1}$$

The entropy is dimensionless and thus, invariant under changes of the units of measurements. For an extension to N-particle systems, see [11].

Fields in QFT are described by the operators $\Psi(\mathbf{r},t)$, where $(\mathbf{r},t)$ is the space-time, and $\Phi(\mathbf{k},t)$ is the spatial Fourier transform of $\Psi(\mathbf{r},t)$. A representation for a system of particles is based on Fock states with occupation number $\left|n_{q_1}, n_{q_2}, , \ldots, n_{q_i}, \ldots n_{q_K}\right\rangle$, where n_{q_i} is the number of particles in a QM state $|q_i\rangle$. The number of particles in a Fock state is then $N = \sum_{i=1}^{K} n_{q_i}$, and a QFT state is described in a Fock space as $|\text{state}\rangle = \sum_m \alpha_m \left|n_{q_1}, n_{q_2}, , \ldots, n_{q_i}, \ldots\right\rangle$, where m is an index over configurations of a Fock state, $\alpha_m \in \mathbb{C}$, and $1 = \sum_m |\alpha_m|^2$. The QFT operators act on a state producing a phase space state $(\Psi(\mathbf{r},t)\,|\text{state}\rangle\,,\,\Phi(\mathbf{k},t)\,|\text{state}\rangle)$. We then define the probability density function for the spatial coordinates as

$$\rho_{\mathrm{r}}^{\mathrm{QFT}}(\mathbf{r},t) = |\Psi(\mathbf{r},t)\,|\text{state}\rangle\,|^2 = \langle\text{state}|\,\Psi^{\dagger}(\mathbf{r},t)\Psi(\mathbf{r},t)\,|\text{state}\rangle\ .$$

Analogously, $\rho_{\mathrm{k}}^{\mathrm{QFT}}(\mathbf{k},t) = |\Phi(\mathbf{k},t)\,|\text{state}\rangle\,|^2 = \langle\text{state}|\,\Phi^{\dagger}(\mathbf{k},t)\Phi(\mathbf{k},t)\,|\text{state}\rangle$.

One may call the coefficients "the wave function" and interpret them as distributions of the information about the position and the space frequency of the state of the field. The QFT coordinate-entropy is then described by (1), where we dropped the superscript QFT, as it will be clear which framework is used, QM or QFT.

In [11], we proved that the coordinate-entropy is invariant under continuous 3D coordinate transformations, continuous Lorentz transformations, and discrete CPT transformations.

Mixed Quantum States

We now extend the entropy (1) to mixed states. Consider a mixed state formed from $m \geq 2$ pure quantum states $\left|\psi_j\right\rangle; j = 1, \ldots, m$, defined by the density matrix $\rho^{\mathrm{M}} = \sum_{j=1}^{m} \lambda_j \left|\psi_j\right\rangle \left\langle\psi_j\right|$, where $\lambda_j > 0$ and $1 = \sum_{j=1}^{m} \lambda_j$. Then, projecting the density matrix onto the quantum coordinate phase space basis yields $\rho_r^{\mathrm{M}}(\mathbf{r}, t) = \langle\mathbf{r}|\,\rho^{\mathrm{M}}\,|\mathbf{r}\rangle = \sum_{j=1}^{m} \lambda_j\, |\psi_j(\mathbf{r}, t)|^2$ and $\rho_k^{\mathrm{M}}(\mathbf{k}, t) = \langle\mathbf{k}|\,\rho^{\mathrm{M}}\,|\mathbf{k}\rangle = \sum_{j=1}^{m} \lambda_j\, |\phi_j(\mathbf{k}, t)|^2$. These are the distributions associated with the observables. We can also consider the distributions $\rho_j(\mathbf{r}, \mathbf{k}, t) = \lambda_j\, |\psi_j(\mathbf{r}, t)|^2\, |\phi_j(\mathbf{k}, t)|^2$, where $1 = \sum_{j=1}^{m} \int \rho_j(\mathbf{r}, \mathbf{k}, t)\ \mathrm{d}^3\mathbf{r}\ \mathrm{d}^3\mathbf{k}$, which account for the quantum coordinate phase space as well as the probabilities associated with specifying the quantum state, namely the probabilities $\lambda_j; j = 1, \ldots, m$. Thus, two different entropies can be considered, one quantifying just the randomness of the observables and the other also quantifying the randomness of specifying the quantum state.

When we are quantifying just the randomness of the observables, then we must consider the probability densities in quantum coordinate phase space to be $\rho_r^{M}(\mathbf{r}, t)$ and $\rho_k^{\mathrm{M}}(\mathbf{k}, t)$ and the differential entropy can be applied to the product of these distributions, i.e., we obtain the entropy

$$\mathrm{S}^{M} = -\int\ \rho_r^{M}(\mathbf{r}, t)\rho_k^{\mathrm{M}}(\mathbf{k}, t)\ \ln\left(\rho_r^{M}(\mathbf{r}, t)\rho_k^{\mathrm{M}}(\mathbf{k}, t)\right)\ \mathrm{d}^3\mathbf{r}\ \mathrm{d}^3\mathbf{k}\,. \tag{2}$$

When however, we attempt to quantify both sources of randomness, the randomness associated with the observables and the randomness associated with the specification of the quantum state, then the density to be considered is $\rho_j(\mathbf{r}, \mathbf{k}, t) =$

$\lambda_j\, |\psi_j(\mathbf{r},t)|^2\, |\phi_j(\mathbf{k},t)|^2$, yielding the entropy

$$
\begin{aligned}
\mathrm{S}^{M.\lambda_j^2} &= -\sum_{j=1}^{m}\int \lambda_j\, |\psi_j(\mathbf{r},t)|^2\, |\phi_j(\mathbf{k},t)|^2\ \ln\left(\lambda_j\, |\psi_j(\mathbf{r},t)|^2\, |\phi_j(\mathbf{k},t)|^2\right)\, \mathrm{d}^3\mathbf{r}\ \mathrm{d}^3\mathbf{k} \\
&= -\sum_{j=1}^{m}\lambda_j \ln\lambda_j + \sum_{j=1}^{m}\lambda_j\, S_j\,,
\end{aligned}
\tag{3}
$$

where $S_j = -\int |\psi_j(\mathbf{r},t)|^2\ \ln|\psi_j(\mathbf{r},t)|^2\ \mathrm{d}^3\mathbf{r} - \int |\phi_j(\mathbf{r},t)|^2\ \ln|\phi_j(\mathbf{r},t)|^2\ \mathrm{d}^3\mathbf{k}$ is the entropy of each pure state.

This entropy has two terms: the von Neumann entropy and the weighted average value of the entropies of the observables for each pure state, weighted by the mixed coefficients λ_j^2. Clearly, the proposed entropy is larger than the von Neumann entropy.

Our proposed entropy for mixed states also differs from Wehrl entropy because it is based on a probability distribution of the observables and not on a quasiprobability distribution that lacks probability properties needed to characterize exactly the randomness of the observables.

One can interpret both entropies (2) and (3) as different generalizations to mixed states of the proposed entropy (1). When the mixed state is reduced to one pure state, with $m = 1$, both reduce to the entropy (1).

In this paper we will focus on pure quantum states and leave as future research to extend the study to mixed states.

Spin-Entropy

The DOFs associated with the spin are captured by a vector or a bispinor representation of the states in both frameworks. It is not possible to know simultaneously the spin of a particle in all three dimensional directions, and this uncertainty, or randomness, was exploited in the Stern–Gerlach experiment [13] to demonstrate the quantum nature of the spin. We explore elsewhere [12] the entropy associated with the quantum spin phase space.

THE MINIMUM ENTROPY VALUE

The third law of thermodynamics establishes 0 as the minimum classical entropy. However, the minimum of the quantum entropy must be positive due to the uncertainty principle's lower bound. Let $\theta(x)$ be 1 for positive x and 0 elsewhere.

Theorem 1. *The minimum entropy of a particle with spin s is* $3(1+\ln\pi)+\theta(s)\ln 2\pi$.

Proof. The entropy is the sum of the coordinate-entropy and the spin-entropy. The coordinate-entropy (1) is $\mathrm{S_r} + \mathrm{S_k}$. Due to the entropic uncertainty principle $\mathrm{S_r} + \mathrm{S_k} \geq 3\ln \mathrm{e}\pi$ as shown in [1, 2, 15], with $\mathrm{S_k} = \mathrm{S_p} - 3\ln\hbar$. To complete the proof, note that in [11] we showed that the minimum spin-entropy is $\theta(s)\ln 2\pi$. □

Higgs bosons in coherent states have the lowest possible entropy $3(1+\ln\pi)$.

The dimensionless element of volume of integration to define the entropy will not contain a particle unless $\mathrm{d}^3\mathbf{r}\;\mathrm{d}^3\mathbf{k} \geq 1$, due to the uncertainty principle, and this may be interpreted as a necessity of discretizing the phase space. We note that the minimum entropy of the discretization of (1) is also $3(1+\ln\pi)$, as shown in [7].

QCURVES AND ENTROPY-PARTITION

We introduce the concept of a QCurve to specify a curve (or path) in a Hilbert space parametrized by time. In QM a QCurve is represented by a triple $\left(|\psi_0\rangle, U(t), \delta t\right)$ where $|\psi_0\rangle$ is the initial state, $U(t) = \mathrm{e}^{-\mathrm{i}\frac{H}{\hbar}t}$ is the evolution operator, and $[0, \delta t]$ is the time interval of the evolution. Of course, one may also represent the initial state by a triple $\left(\rho_0, U(t), \delta t\right)$, where $\rho_0 = |\psi_0\rangle\langle\psi_0|$ is the density matrix. Alternatively, we can represent the initial state in the quantum coordinate phase space by $(\langle \mathbf{r}|\psi_0\rangle, \langle \mathbf{k}|\psi_0\rangle)$ or by $(\langle \mathbf{r}|\rho_0|\mathbf{r}\rangle, \langle \mathbf{k}|\rho_0|\mathbf{k}\rangle)$, and in QFT by $(\Psi(\mathbf{r},0)|\text{state}\rangle, \Phi(\mathbf{k},0)|\text{state}\rangle)$, or via the density operators $(\langle\text{state}|\rho_r(\mathbf{r},0)|\text{state}\rangle, \langle\text{state}|\rho_k(\mathbf{k},0)|\text{state}\rangle)$, with $\rho_r(\mathbf{r},0)=\Psi^\dagger(\mathbf{r},0)\Psi(\mathbf{r},0)$ and $\rho_k(\mathbf{k},0)=\Phi^\dagger(\mathbf{k},0)\Phi(\mathbf{k},0)$. We will use any of these representations to describe a QCurve as more convenient for manipulations for the problem at hand.

Definition 1 (Partition of $\mathcal{E}$)**.** Let $\mathcal{E}$ to be the set of all the QCurves. We define a partition of $\mathcal{E}$ based on the entropy evolution into four blocks:

$\mathcal{C}$**:** Set of the QCurves for which the entropy is a constant.

$\mathcal{I}$**:** Set of the QCurves for which the entropy is increasing, but it is not a constant.

$\mathcal{D}$**:** Set of the QCurves for which the entropy is decreasing, but it is not a constant.

$\mathcal{O}$**:** Set of the oscillating QCurves, with the entropy strictly increasing in some subinterval of $[0,\delta t]$ and strictly decreasing in another subinterval of $[0,\delta t]$.

It is straightforward to show that all stationary states are in $\mathcal{C}$ (see [11]).

The Coordinate-Entropy of Coherent States Increases With Time

Coherent states, represented by state $|\alpha\rangle$, are eigenstates of the annihilator operator. The 1D quantum phase space of observable variables (x,p) can be constructed by the unitary operator $U(x_0,p_0)=e^{\frac{i}{\hbar}(x_0X-p_0P)}$ applied to "zero-state" $|x=0,p=0\rangle$, i.e., they can be constructed as $|\alpha\rangle=|x_0,p_0\rangle=e^{\frac{i}{\hbar}(x_0X-p_0P)}|0,0\rangle$, where $\alpha=x_0+ip_0$. Projecting the state to position space yields $\psi_\alpha(x)=\langle x|\alpha\rangle=\frac{e^{-\frac{p_0^2}{2}}}{\pi^{\frac{1}{4}}}e^{-\frac{1}{2}\left(x-\sqrt{2}\alpha\right)^2}$, where $\alpha=\frac{1}{\sqrt{2}}(x_0+ip_0)$. Squeeze states extend coherent states to all eigenstate solutions of the annihilator operator by allowing different variances to the Gaussian solution, and together their representation in 3D position and momentum space are

$$\psi_{\mathrm{k}_0}(\mathbf{r}-\mathbf{r}_0) = \frac{1}{2^3\pi^{\frac{3}{2}}(\det\boldsymbol{\Sigma})^{\frac{1}{2}}}\,\mathcal{N}\left(\mathbf{r}\mid\mathbf{r}_0,\boldsymbol{\Sigma}\right)\,\mathrm{e}^{\mathrm{i}\mathbf{k}_0\cdot\mathbf{r}}\,,$$
$$\Phi_{\mathrm{r}_0}(\mathbf{k}-\mathbf{k}_0) = \frac{1}{2^3\pi^{\frac{3}{2}}(\det\boldsymbol{\Sigma}^{-1})^{\frac{1}{2}}}\,\mathcal{N}\left(\mathbf{k}\mid\mathbf{k}_0,\boldsymbol{\Sigma}^{-1}\right)\,\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{r}_0}\,, \tag{4}$$

where $\boldsymbol{\Sigma}$ is the spatial covariance matrix. We will continue to refer to these states as coherent, with the understanding that we are including squeezed states and that replacing the general covariance $\boldsymbol{\Sigma}$ by I reduces to the formal definition of coherent states. The foundational material follows from most common textbooks, e.g., [6, 10, 20, 24].

In [11] we proved that for a QCurve with an initial coherent state (4) and evolving according to the energy $\hbar\omega(\mathrm{k}) = \hbar\sqrt{\mathbf{k}^2c^2+\left(\frac{mc^2}{\hbar}\right)^2}$, the entropy evolves as $3(1+\ln\pi)+\frac{1}{2}\ln\det\left(\mathbf{I}+t^2(\boldsymbol{\Sigma}^{-1}\mathbf{H})^2\right)$, where

$$\mathbf{H}_{ij} = \mathbf{H}_{ij}(\mathbf{k}_0) = \frac{\hbar}{m}\left(1+\left(\frac{\hbar k_0}{mc}\right)^2\right)^{-\frac{3}{2}}\left[\delta_{i,j}\left(1+\left(\frac{\hbar k_0}{mc}\right)^2\right)-\left(\frac{\hbar k_{0i}}{mc}\right)\left(\frac{\hbar k_{0j}}{mc}\right)\right]\,,$$

and $\mathbf{H}$ is positive definite. Thus, the QCurve is in $\mathcal{I}$. This suggests that quantum physics has an inherent dispersion mechanism to increase entropy for free fermion particles. Note that for coherent states of photons, no dispersion occurs as the electromagnetic Hamiltonian is non-dispersive.

Time Reflection as a Mechanism to Convert QCurves in $\mathcal{I}$ to $\mathcal{D}$ and Vice-Versa

We consider a time-independent Hamiltonian and investigate the discrete symmetries C and P, and Time Reflection, the augmentation of Time Reversal with Time Translation, i.e., the classical mapping $t \mapsto t' = -t + \delta t$. We define the Time Reflection quantum field, T_δ, as $\Psi^{\mathrm{T}_\delta}(\mathbf{r}, -t+\delta t) = \mathcal{T}\Psi(\mathbf{r},t) = T\Psi^*(\mathbf{r},t)$, where

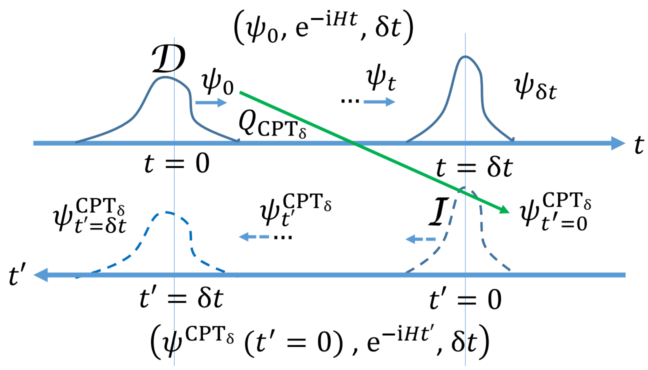


Figure 1. A visualization of the Time Reflection Theorem. (i) Axis t: A QCurve $e_1 = \big(\psi_0(\mathbf{r}), \mathrm{e}^{-\mathrm{i}Ht}, \delta t\big)$. (ii) Axis $t' = \delta t - t$: The antiparticle QCurve is created as $e_2 = Q_{\mathrm{CPT}_\delta}(e_1) = \big(\psi^{\mathrm{CPT}_\delta}(-\mathbf{r}, t' = 0), \mathrm{e}^{-\mathrm{i}Ht'}, \delta t\big)$. Axis t' shows the evolution as going forward in time t'. The evolution of $\psi^{\mathrm{CPT}_\delta}(-\mathbf{r}, t') = \eta\gamma^5\,(\Psi^\dagger)^\mathsf{T}(\mathbf{r}, \delta t - t')$ is mirroring the evolution of $\psi(\mathbf{r}, t)$, with $t = t'$ evolving from 0 to δt. If $e_1 \in \mathcal{D}$, then $e_2 \in \mathcal{I}$.

$\Psi^\mathrm{T}(\mathbf{r}, -t) = \mathcal{T}\Psi(\mathbf{r}, t) = T\Psi^*(\mathbf{r}, t)$ is the Time Reversal transformation.

Note that in contrast to the case of Time Reversal, the entropies associated with $\Psi(\mathbf{r}, t)$ and $\Psi^{\mathrm{T}_\delta}(\mathbf{r}, t)$ are generally not equal. Thus, an instantaneous Time Reflection transformation will cause entropy changes.

Definition 2 (Q_{CPT_δ})**.** Let $\gamma^5 = \mathrm{i}\gamma^0\gamma^1\gamma^2\gamma^3$ and η a phase factor. Then Q_{CPT_δ} maps $\big(\psi(\mathbf{r}, 0), U(t), \delta t\big) \mapsto \big(\psi^{\mathrm{CPT}_\delta}(-\mathbf{r}, 0), U(t), \delta t\big)$, where

$$\psi^{\mathrm{CPT}_\delta}(-\mathbf{r}, 0) = \eta\, CPT\, \overline{\Psi}^\mathsf{T}(\mathbf{r}, -\delta t) = \eta\gamma^5\,(\Psi^\dagger)^\mathsf{T}(-\mathbf{r}, \delta t)\,.$$

We proved in [11] a Time Reflection Theorem stating that when $e_1 = (\psi(\mathbf{r}, t_0), U(t), \delta t)$ is a QCurve solution to a QFT (under some basic conditions satisfied by the standard model), then $e_2 = Q_{\mathrm{CPT}_\delta}(e_1)$ is also a solution to such a QFT. Furthermore, under Q_{CPT_δ}, $\mathcal{C}$, $\mathcal{I}$, $\mathcal{O}$, $\mathcal{D}$ are the reflections of $\mathcal{C}$, $\mathcal{D}$, $\mathcal{O}$, $\mathcal{I}$, respectively. The case when $e_1 \in \mathcal{D}$, and therefore $e_2 \in \mathcal{I}$, is depicted in Figure 1, showing a relation between a particle and an antiparticle.

Entropy Oscillations

Consider a Hamiltonian $H' = H + H^{\mathrm{I}}$, where $|H^{\mathrm{I}}| \ll |H|$, and the initial eigenstate $\left|\psi_{E_i}\right\rangle$ of H associated with the eigenvalue $E_i = \hbar\omega_i$. The time evolution of $\left|\psi_{E_i}\right\rangle$ is

$$|\psi_t\rangle = \mathrm{e}^{-\mathrm{i}\frac{(H+H^{\mathrm{I}})}{\hbar}t} \left|\psi_{E_i}\right\rangle = \sum_{k=1}^{n} \alpha_k(t) \left|\psi_{E_k}\right\rangle ,$$

where n is the number of the eigenvectors of H. Fermi's golden rule [8, 9] approximates the coefficients of transition for $k \neq i$ and short time intervals by

$$\alpha_k(t) \approx \frac{H^{\mathrm{I}}_{i,k}}{\hbar(\omega_i - \omega_k)} \left(-2\sin^2\left(\frac{(\omega_i - \omega_k)t}{2}\right) + \mathrm{i}\sin\left((\omega_i - \omega_k)t\right)\right) .$$

Theorem 2 (Entropy Oscillations)**.** *Consider the QCurve* $\left(\left|\psi_{E_i}\right\rangle, U(t) = e^{-\mathrm{i}\frac{(H+H^{\mathrm{I}})}{\hbar}t}, T\right)$ *with* $\hbar\omega_1$ *the ground state value of* H *and* $T = \frac{2\pi}{|\omega_i - \omega_1|}$. *Assume that* $|\alpha_1(t)|^2, |\alpha_i(t)|^2 \gg |\alpha_k(t)|^2$ *for* $k \neq 1, i$ *and* $t \in [0, T]$. *Then the QCurve is in* $\mathcal{O}$.

Proof. With the theorem's assumptions, we can approximate the position and the momentum probability densities associated with $|\psi_t\rangle$ by

$$\rho_{\mathrm{r}}(\mathbf{r}, t) \approx \left|\sqrt{1 - |\alpha_1(t)|^2} \left\langle \mathbf{r} \middle| \psi_{E_i} \right\rangle + \alpha_1(t) \left\langle \mathbf{r} \middle| \psi_{E_1} \right\rangle\right|^2 ,$$
$$\rho_{\mathrm{k}}(\mathbf{k}, t) \approx \left|\sqrt{1 - |\alpha_1(t)|^2} \left\langle \mathbf{k} \middle| \psi_{E_i} \right\rangle + \alpha_1(t) \left\langle \mathbf{k} \middle| \psi_{E_1} \right\rangle\right|^2 .$$

The time coefficients are the same for $\rho_{\mathrm{r}}(\mathbf{r}, t)$ and $\rho_{\mathrm{k}}(\mathbf{k}, t)$, and they all return to the same values simultaneously after a period of T, and so the entropy will return to its previous value too. As the entropy is not a constant, it must be oscillating. $\square$

Thus, when Fermi's golden rule can be applied, the coefficients of the transition probabilities of the unitary evolution of a state oscillate, and the entropy associated with the evolution of such a state will also oscillate with the same period.

PHYSICAL SCENARIOS WITH PARTICLE CREATION

A Two-Particle Collision

Consider a two-fermions or a two-massive-bosons system

$$|\psi_t\rangle = \frac{1}{\sqrt{C_t}}\left(\left|\psi_t^1\right\rangle\left|\psi_t^2\right\rangle \mp \left|\psi_t^2\right\rangle\left|\psi_t^1\right\rangle\right) ,$$

where C_t is the normalization constant that may evolve over time and the signs "$\mp$" represent fermions ("$-$") and bosons ("$+$"). When $\left|\psi_t^1\right\rangle$ and $\left|\psi_t^2\right\rangle$ are orthogonal to each other, $C_t = 2$. Projecting on $\langle \mathbf{r}_1|\,\langle \mathbf{r}_2|$ and on $\langle \mathbf{k}_1|\,\langle \mathbf{k}_2|$,

$$\begin{aligned}
\psi(\mathbf{r}_1,\mathbf{r}_2,t) &= \frac{1}{\sqrt{C_t}}\left(\psi_1(\mathbf{r}_1,t)\psi_2(\mathbf{r}_2,t) \mp \psi_1(\mathbf{r}_2,t)\psi_2(\mathbf{r}_1,t)\right) ,\\
\psi(\mathbf{k}_1,\mathbf{k}_2,t) &= \frac{1}{\sqrt{C_t}}\left(\phi_1(\mathbf{k}_1,t)\phi_2(\mathbf{k}_2,t) \mp \phi_1(\mathbf{k}_2,t)\phi_2(\mathbf{k}_1,t)\right) .
\end{aligned}$$

From [11], the entropy of the two-particle system, discarding the spin-entropy which is constant throughout the collision, is then

$$\begin{aligned}
S\left(\left|\psi_t^1\right\rangle,\left|\psi_t^2\right\rangle\right) = &-\int \mathrm{d}^3\mathbf{r}_1 \int \mathrm{d}^3\mathbf{r}_2\, \rho_\mathrm{r}(\mathbf{r}_1,\mathbf{r}_2,t)\ln\rho_\mathrm{r}(\mathbf{r}_1,\mathbf{r}_2,t)\\
&-\int \mathrm{d}^3\mathbf{k}_1 \int \mathrm{d}^3\mathbf{k}_2\, \rho_\mathrm{k}(\mathbf{k}_1,\mathbf{k}_2,t)\ln\rho_\mathrm{k}(\mathbf{k}_1,\mathbf{k}_2,t) .
\end{aligned}$$

Consider a collision of two particles, each one described by an initial coherent state with position variance σ^2 centered at c_1 and c_2 and moving towards each other along the x-axis with center momenta $p_0 = \hbar k_0$ and $-p_0$. They can be represented in position and momentum space as

$$\begin{aligned}
\Psi_1(x,t) &= \frac{\mathrm{e}^{-\mathrm{i}k_0 v_p(k_0)\,t}}{Z_1}\,\mathcal{N}\left(x \mid c_1 + v_g(k_0)\,t, \sigma^2 + \mathrm{i}\,t\,\mathcal{H}(k_0)\right)\mathrm{e}^{\mathrm{i}k_0 x}\,,\\
\Psi_2(x,t) &= \frac{\mathrm{e}^{-\mathrm{i}k_0 v_p(k_0)\,t}}{Z_1}\,\mathcal{N}\left(x \mid c_2 - v_g(k_0)\,t, \sigma^2 + \mathrm{i}\,t\,\mathcal{H}(-k_0)\right)\mathrm{e}^{-\mathrm{i}k_0 x}\,,\\
\Phi_1(k,t) &= \frac{\mathrm{e}^{-\mathrm{i}t\,v_p(k_0)k_0}}{Z_{k_0}}\,\mathcal{N}\left(k \mid k_0, (\sigma^2 + \mathrm{i}\,t\,\mathcal{H}(k_0))^{-1}\right)\mathrm{e}^{\mathrm{i}(k-k_0)\left(c_1+v_g(k_0)\,t\right)}\,,\\
\Phi_2(k,t) &= \frac{\mathrm{e}^{-\mathrm{i}t\,v_p(k_0)k_0}}{Z_{k_0}}\,\mathcal{N}\left(k \mid -k_0, (\sigma^2 + \mathrm{i}\,t\,\mathcal{H}(-k_0))^{-1}\right)\mathrm{e}^{\mathrm{i}(k+k_0)\left(c_2-v_g(k_0)\,t\right)}\,. \quad (5)
\end{aligned}$$

Figure 2 shows that when the two particles are far apart, the entropy of the system is close to the sum of the two individual entropies, with each one increasing over time. The spatial entanglement decreases the uncertainty, and therefore the entropy too. The competition between the increase of the entropy of the individual particles and the decrease of the entropy due to entanglement results in an oscillation and the decrease in the total entropy when the two particles are close to each other.

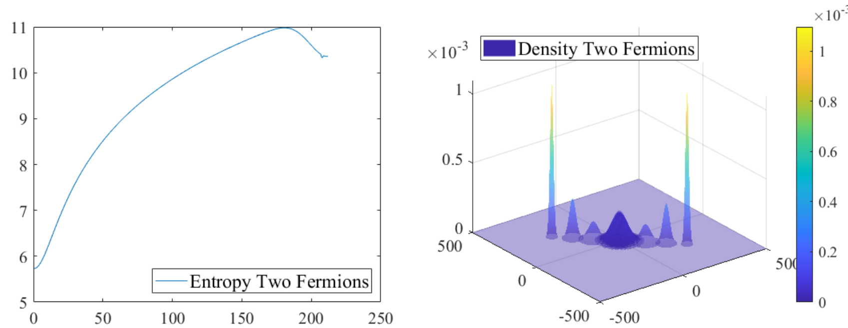
The Hydrogen Atom and Photon Emission

The QED Hamiltonian for the hydrogen atom is

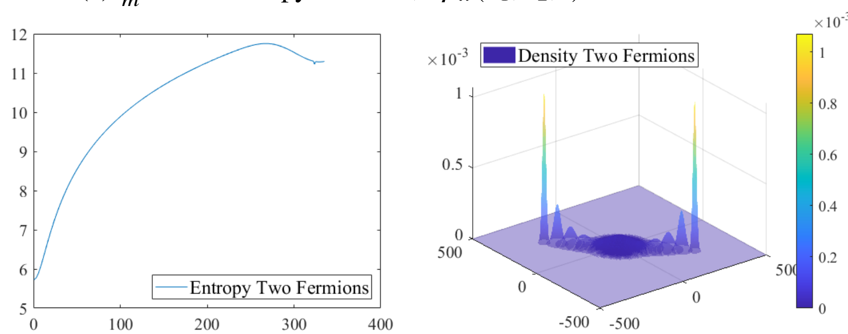
$$H(p,r,q) = \sum_{i=1}^{3}\frac{\left(p^i - \frac{\mathrm{e}}{c}A^i(q)\right)^2}{2m} - \frac{\mathrm{e}^2}{r} + \sum_{\lambda=1}^{2}\hbar\omega_q\, a_\lambda^\dagger(q)\, a_\lambda(q)\,,$$

where the photon's helicity λ is 1 or 2, $\omega_q = |q|c$, the creation and the annihilation operators of photons satisfy $[a_\lambda(p), a_{\lambda'}^\dagger(q)] = \delta_{\lambda,\lambda'}\delta(p-q)$, and the electromagnetic vector potential is

$$\tilde{A}^i(q) = \sqrt{2\pi\hbar c^2}\sum_{\lambda=1}^{2}\frac{1}{\sqrt{\omega_q}}\left(\epsilon_\lambda^i(q)\, a_\lambda(q) + \epsilon_\lambda^{*\mathrm{i}}(q)\, a_\lambda^\dagger(q)\right)\,,$$



(a) $\frac{\hbar}{m} = 1$: Entropy vs. time; $\rho_x(x_1, x_2, t)$ overlaid over time



(b) $\frac{\hbar}{m} = 0.5$: Entropy vs. time; $\rho_x(x_1, x_2, t)$ overlaid over time

Figure 2. Collision of two fermions with individual amplitudes (5), parameters $k_0 = 1$, $c_2 = -c_1 = 300$, speed of light $c = 1$, a grid of 1 000 points for x_1, x_2, k_1, k_2. The left column shows entropy vs. time. The right column shows snapshots of the density at initial time, final time, and intervals of 100 time units, overlaid on single plots. The z-axis represents the density, and the x-y axes represent the x_1-x_2 values. As the particles approach each other, their individual densities disperse, the maximum values are reduced, and the entropy increases. Only when the particles are close to each other, the interference reduces the total entropy.

and in the Coulomb Gauge ($\nabla \cdot A = 0$), for $q = |q|(\sin\theta_q \cos\phi_q, \sin\theta_q \sin\phi_q, \cos\theta_q)$, the polarizations satisfy $\epsilon_1(q) = (\cos\theta_q \cos\phi_q, \cos\theta_q \sin\phi_q, \sin\theta_q)$ and $\epsilon_2(q) = (-\sin\phi_q, \cos\phi_q, 0)$.

The state of the atom can be described by $|n, l, m\rangle_{\mathrm{e}^-} |q, \lambda\rangle_\gamma$, where n, l, m are the quantum numbers of the electron e^-, and q and λ are the momentum and the helicity of the photon γ. We next consider the Lyman-alpha transition, $|n = 2, l = 1, m = 0\rangle |0\rangle \to |n = 1, l = 0, m = 0\rangle |q, \lambda\rangle$ with the emission of a photon with wavelength $\lambda \approx 121.567 \times 10^{-9}$ m.

We first evaluate the electron's entropy at both states $|n = 2, l = 1, m = 0\rangle$ and $|n = 1, l = 0, m = 0\rangle$. For simplicity, we consider the Schrödinger approximation to describe the electron state with the energy change in this transition of $\Delta E_{n=2\to n=1} \approx -\left(\frac{1}{2^2} - 1\right) \times 13.6\,\text{eV} = 10.2\,\text{eV}$. We now compute the difference between the final and the initial state entropy following three steps.

(i) The position probability amplitudes described in [3] and the associated entropies are

$$\psi_{2,1,0}(\rho,\theta,\phi) = \frac{1}{\sqrt{32\pi}}\left(\frac{1}{a_0}\right)^{\frac{3}{2}} \rho e^{-\frac{\rho}{2}}\cos(\theta) \;\rightarrow\; \mathrm{S}_{\mathrm{r}}(\psi_{2,1,0}) \approx 6.120 + \ln\pi + 3\ln a_0\,,$$

$$\psi_{1,0,0}(\rho,\theta,\phi) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-\rho} \;\rightarrow\; \mathrm{S}_{\mathrm{r}}(\psi_{1,0,0}) \approx 3.000 + \ln\pi + 3\ln a_0\,,$$

where $a_0 \approx 5.292 \times 10^{-11}$ m is the Bohr radius, and $\rho = r/a_0$.

(ii) The momentum probability amplitudes described in [3] and the associated entropies are

$$\begin{aligned}
\Phi_{2,1,0}(p,\theta_p,\phi_p) &= \sqrt{\frac{128^2}{2\pi p_0^3}\,\frac{p}{p_0}}\left(1+\left(2\frac{p}{p_0}\right)^2\right)^{-3}\cos(\theta_p)\,,\\
&\rightarrow\quad \mathrm{S}_p(\Phi_{2,1,0}) \approx 0.042 + 3\ln p_0\,,\\
\Phi_{1,0,0}(p,\theta_p,\phi_p) &= \sqrt{\frac{32}{\pi p_0^3}}\left(1+\left(\frac{p}{p_0}\right)^2\right)^{-2}\,,\\
&\rightarrow\quad \mathrm{S}_p(\Phi_{1,0,0}) \approx 2.422 + 3\ln p_0\,,
\end{aligned}$$

where $p_0 = \hbar/a_0$.

(iii) Therefore, $\Delta \mathrm{S}_{2,1,0\to 1,0,0} = \mathrm{S}_{\mathrm{r}}(\psi_{1,0,0}) + \mathrm{S}_p(\Phi_{1,0,0}) - \mathrm{S}_{\mathrm{r}}(\psi_{2,1,0}) - \mathrm{S}_p(\Phi_{2,1,0}) \approx$

$-0.740\,.$

Thus, the entropy of the electron is reduced by approximately 0.740 during the transition $|n=2, l=1, m=0\rangle \;\rightarrow\; |n=1, l=0, m=0\rangle$.

We next evaluate the entropy associated with the randomness in the emission of the photon. Due to energy conservation, the energy must satisfy $|q|c \approx 10.2\,\text{eV}$, where c is the speed of light. The associated energy uncertainty is very small. The main randomness for the photon is in specifying the direction of the emission. The angular momentum of the electron along z ($m=0$) does not change between $|n=2, l=1, m=0\rangle$ and $|n=1, l=0, m=0\rangle$. The spin 1 of the photon is along its motion, and conserves the total angular momentum of the system. Thus, to conserve angular momentum along z, the photon must be moving perpendicularly to the z axis, that is, $\theta_q = \frac{\pi}{2}$, and so the polarization vectors must be $\epsilon_1(q) = (0,0,1)$ and $\epsilon_2(q) = (-\sin\phi_q, \cos\phi_q, 0)$. The angle ϕ_q is completely unknown, with the entropy $\ln 2\pi$. Then we observe that the entropy increases, as

$$\Delta \mathrm{S}_{|n=2,l=1,m=0\rangle|0\rangle \rightarrow |n=1,l=0,m=0\rangle|q,\lambda\rangle} \approx \ln 2\pi - 0.740 = 1.098\,.$$

Consider now an apparent time-reversing scenario in which an apparatus emitted photons with energy $E_\gamma = \hbar|\omega_{n=2,l=1,m=0} - \omega_{n=1,l=0,m=0}|$ to strike a hydrogen atom with its electron in the ground state. The photon had to follow a precise direction towards the atom, and a very small uncertainty in the direction implies low photon entropy. Once the atom absorbs the photon, the energy of the electron in the ground state suffices for a jump into an excited state. The entropy increases again, as the entropy of the excited state is greater than the entropy of the ground state (accounting for the low photon entropy).

AN ENTROPY LAW AND A TIME ARROW

In classical statistical mechanics, the entropy provides a time arrow through the second law of thermodynamics [5]. We have shown that due to the dispersion property of the fermionic Hamiltonian, some states, such as coherent states, evolve with an increasing entropy. However, current quantum physics is time reversible, and we have just studied in the previous section several scenarios where the entropy oscillates. This study lead us to think that entropy oscillations do not in fact occur in nature, and instead and inspired by the second law of thermodynamics, we conjecture

Law (The Entropy Law)**.** *The entropy of a quantum system is an increasing function of time.*

Let us review some of the physical scenarios where oscillations may not take place:

1. A high-speed collision $e^+ + e^- \to 2\gamma$ may produce new particles instead of allowing the entropy to decrease (see Figure 2).

2. According to QED, and due to photon fluctuations of the vacuum, the state of an electron in an excited state of the hydrogen atom is in a superposition with the ground state, and by Theorem 2 the entropy would decrease within a time interval $2\pi/|\omega_{n=2,l=1,m=0} - \omega_{n=1,l=0,m=0}|$. Instead, the electron jumps to the ground state and a photon is created/emitted, increasing the entropy.

3. We speculate that the QCurve of a neutral K meson (kaon K^0) [4], $e_0 = (\psi_0(\mathbf{r}), U(t), \frac{2\pi}{\Delta w})$, is in $\mathcal{O}$. Then, a K^0 particle in state $\psi_0(\mathbf{r})$ evolves with increasing entropy until, say at time T, it enters the remaining segment of QCurve $e_T = (\psi_T(\mathbf{r}), U(t), [T, \frac{2\pi}{\Delta w}])$ in $\mathcal{D}$. To block such a decrease (forbidden by the entropy law), a transformation takes place, with quarks exchanging bosons to transform $\mathrm{K}^0 \mapsto \bar{\mathrm{K}}^0$ to create an antiparticle's QCurve e_1 in $\mathcal{I}$.

We conjecture that the entropy law is the trigger for those particles' creation. In [11] we studied the spin-entropy in more depth, and this law would impact on the issue of which spin state evolutions would be physically allowed.

CONCLUSIONS

Capturing all the information of a quantum state requires the specifying of the parameters associated with the DOFs of a quantum state as well as as the intrinsic randomness of the quantum state. We proposed an entropy defined in the quantum phase spaces. We defined quantum phases spaces to be the space of all possible states projected in the position and spatial frequency basis. This definition of the entropy and quantum phase spaces possesses desirable properties, including invariance in special relativity, and invariance under CPT transformations. We argued that it is necessary to consider both projections in order to capture all the randomness of the observables.

We characterized the behaviors of all quantum states according to their entropy evolution. To this end, we introduced a QCurve structure, a triple representing the initial state, the unitary evolution operator, and a time interval. We partitioned the set of all the QCurves into four blocks, characterized by the entropy during an evolution. A QCurve is in $\mathcal{C}$ if the entropy is a constant, in $\mathcal{I}$ if it is increasing, in $\mathcal{D}$ if it is decreasing, and in $\mathcal{O}$ if it is oscillating.

We showed that due to the dispersion property of a fermionic Hamiltonian, QCurves of initially coherent states are in $\mathcal{I}$. We extended the CPT transformation to allow for Time Reflection, consequently mapping $\mathcal{C}$, $\mathcal{I}$, $\mathcal{O}$, $\mathcal{D}$, to $\mathcal{C}$, $\mathcal{D}$, $\mathcal{O}$, $\mathcal{I}$, respectively. Then we revisited Fermi's golden rule, discussing its relation to QCurves in $\mathcal{O}$. We showed that the entropy increases when an electron in an excited state of the hydrogen atom falls to the ground state emitting a photon. We studied the collision of two particles, each in a coherent state. The entropy of each particle alone is increasing, but as they approach each other, an entropy oscillation can occur in the two-particle system due to their entanglement.

We observe that many interesting particle- or atomic-physics phenomena seem to be described by scenarios where QCurves are in $\mathcal{O}$, such as (i) decay of atoms (Fermi's golden rule), (ii) electrons in excited states of atoms that transition to the ground state causing emission of radiation, (iii) particle oscillations (e.g., neutrinos and neutral kaons), and (iv) collision of particles that lead to annihilation of particles and creation of new particles.

We conjectured an entropy law that would trigger the formation of the states with particle creation or annihilation. We considered states whose evolution is described by Fermi's golden rule, and so such QCurves are in $\mathcal{O}$. Fermi's golden rule describes a unitary evolution of a state that at any time is in a superposition of states that do create or anhilate particles with the ones that do not create nor anhilate particles, albeit in the case that we are considering with larger coefficients for formers states. Our proposed entropy law determines that the event of particle creation happens, and offers causality, time irreversibility, and deterministic reasoning for the state transition and the creation of particles.

ACKNOWLEDGEMENT

This paper is partially based upon work supported by both the National Science Foundation under Grant No. DMS-1439786 and the Simons Foundation Institute Grant Award ID 507536 while the first author was in residence at the Institute for Computational and Experimental Research in Mathematics in Providence, RI, during the spring 2019 semester "Computer Vision" program.

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