Quantum Information Physics I

TR2021-996

Davi Geiger and Zvi M. Kedem

Courant Institute of Mathematical Sciences

New York University, New York, New York 10012

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 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's entropy [18] 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). Therefore, it is not possible to start with von Neumann's entropy if one wants to assign an entropy that measures the randomness of a one-particle state, and then extend it to multiple particles and a quantum field.

In classical physics, Boltzmann entropy and Gibbs entropy and their respective H-theorems [13] are formulated in the 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 [16]. 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). 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 measuring total randomness.

To be useful, the entropy in quantum physics must (i) account for all the DOFs of a state, (ii) be a measure of randomness of such a state, and (iii) be invariant under the applicable transformations. We propose an entropy defined in phase spaces associated with the DOFs and that satisfies those conditions. 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.

The study of the QCurves in the blocks of the partition leads us to conjecture that there is an entropy law, whereby entropy never decreases, applicable to all particle physics.

QUANTUM ENTROPY IN 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 $|\psi\rangle_t$ 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, $|\mathbf{r}\rangle$ or $|\mathbf{p}\rangle$, is sufficient to recover the other one via a Fourier transform. As illustrated by the uncertainty principle, the randomness of the coordinates of a particle is described in the coordinate phase space ($\psi(\mathbf{r},t) = \langle \mathbf{r}|\psi_t\rangle$, $\phi(\mathbf{p},t) = \langle \mathbf{p}|\psi_t\rangle$). By Born's rule, $\rho_{\mathrm{r}}(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2$ and $\rho_p(\mathbf{p},t) = |\tilde{\phi}(\mathbf{p},t)|^2$ are the probability densities of the phase-space representation of the state.

Motivated by Gibbs [13] and Jaynes [15], we will define S, the coordinate-entropy of a particle. Let $\mathbf{k} = \frac{1}{\hbar}\mathbf{p}$ be the spatial frequency, $\rho_k(\mathbf{k},t) = \frac{1}{\hbar^3}\rho_p(\mathbf{p},t)$ the associated probability density, $\mathrm{S_r} = -\int \rho_{\mathrm{r}}(\mathbf{r},t) \ln \rho_{\mathrm{r}}(\mathbf{r},t)\ \mathrm{d}^3\mathbf{r}$; and analogously for $\mathrm{S_k}$. Then we define

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

The entropy is dimensionless and 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 $\left|n_{q_1}, n_{q_2}, , \ldots, n_{q_i}, \ldots\right\rangle$, 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.

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 [12] to demonstrate the quantum nature of the spin.

We characterize the spin phase space by considering simultaneously a spin state along x, y, and z directions, i.e., a spin state $|\xi\rangle$ is represented in spin phase space as $(|\xi\rangle_x, |\xi\rangle_y, |\xi\rangle_z)$, and an spin-entropy term derived from the probability distribution associated with each state direction is added to produce the spin-entropy. The derivation of a spin-entropy for massive particles with spin $s = \frac{1}{2}, 1$ is presented in [11]. Clearly, an eigenstate $|\xi\rangle_z$ does not imply that the entropy is 0 due to the possible uncertainties in $|\xi\rangle_x$ and $|\xi\rangle_y$. Note however, that preparing a system to align a spin state with a particular direction, say an eigenstate $|\xi\rangle_z$, as it is done in many experiments with spin (e.g., [12]), implies the knowledge of one of the spin directions. Thus its spin-entropy must have been reduced by the preparation. This topic as well as the entanglement of two spin $s = \frac{1}{2}$ particles is further studied in [11]. For particles with $s = 0$ (scalar fields) the spin entropy is 0. A massless field with $s = 1$ is described by the gauge field $A^\mu(\mathbf{r}, t)$, a vector under Lorentz transformation. In this case, the spin uncertainty is reflected by the two polarization vectors and is derived in a later section that considers the photon emission in the hydrogen atom.

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* $s = 0, \frac{1}{2}, 1$ *is* $3(1 + \ln \pi) + 2\theta(s) \ln 2$.

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, 14], with $\mathrm{S_k} = \mathrm{S_p} - 3 \ln \hbar$. To complete the proof, in [11] we showed that the minimum spin-entropy is $2\theta(s) \ln 2$. □

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, $U(t) = \mathrm{e}^{-\mathrm{i}Ht}$ is the evolution operator, and $[0, \delta t]$ is the time interval of the evolution. Alternatively, we can represent the initial state by $(\langle \mathbf{r}|\psi_0\rangle, \langle \mathbf{k}|\psi_0\rangle)$ and in QFT by $(\Psi(\mathbf{r}, 0)\,|\text{state}\rangle, \Phi(\mathbf{k}, 0)\,|\text{state}\rangle)$.

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 the state $|\alpha\rangle$, the eigenstates of the annihilator operator, yield in position and momentum space representations

$$\begin{aligned}\psi_{\mathrm{k}_0}(\mathbf{r}-\mathbf{r}_0) &= \langle \mathbf{r}|\alpha=0\rangle = \frac{1}{2^3\pi^{\frac{3}{2}}(\det\boldsymbol{\Sigma})^{\frac{1}{2}}}\,\mathcal{N}\left(\mathbf{r}\mid\mathbf{r}_0,\boldsymbol{\Sigma}\right)\,\mathrm{e}^{\mathrm{i}\mathbf{k}_0\cdot\mathbf{r}}\,,\\ \Phi_{\mathrm{r}_0}(\mathbf{k}-\mathbf{k}_0) &= \langle \mathbf{k}|\alpha=0\rangle = \frac{1}{2^3\pi^{\frac{3}{2}}(\det\boldsymbol{\Sigma}^{-1})^{\frac{1}{2}}}\,\mathcal{N}\left(\mathbf{k}\mid\mathbf{k}_0,\boldsymbol{\Sigma}^{-1}\right)\,\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{r}_0}\,,\end{aligned}\tag{2}$$

where $\boldsymbol{\Sigma}$ is the spatial covariance matrix. The foundational material follows from most common textbooks, e.g., [6, 10, 17, 19].

In [11] we proved that for a QCurve with an initial coherent state (2) 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.

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 $\Psi^{\mathrm{T}_\delta}(\mathbf{r},-t+\delta t)=\mathcal{T}\Psi(\mathbf{r},t)=T\Psi^*(\mathbf{r},t)$.

Note that in contrast to the case of Time Reversal, $\Psi^{\mathrm{T}}(\mathbf{r},-t)=\mathcal{T}\Psi(\mathbf{r},t)$, the

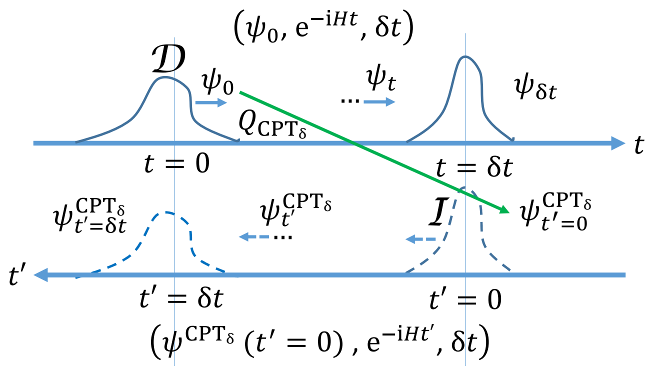


Figure 1. A visualization of the Time Reflection Theorem. (i) Axis t: A QCurve $e_1 = \left(\psi_0(\mathbf{r}), \mathrm{e}^{-\mathrm{i}Ht}, \delta t\right)$. (ii) Axis $t' = \delta t - t$: The antiparticle QCurve is created as $e_2 = Q_{\mathrm{CPT}_\delta}(e_1) = \left(\psi^{\mathrm{CPT}_\delta}(-\mathbf{r}, t' = 0), \mathrm{e}^{-\mathrm{i}Ht'}, \delta t\right)$. 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 $e_2 \in \mathcal{I}$.

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 $\left(\psi(\mathbf{r}, 0), U(t), \delta t\right) \mapsto \left(\psi^{\mathrm{CPT}_\delta}(-\mathbf{r}, 0), U(t), \delta t\right)$, 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 $\mathcal{C}$, $\mathcal{D}$, $\mathcal{O}$, $\mathcal{I}$. 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. □

PHYSICAL SCENARIOS WITH PARTICLE CREATION

A Two-Particle Collision

Consider a two-fermions or a two-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 in 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

$$\begin{aligned}
\Psi_1(x,t) &= \frac{\mathrm{e}^{-\mathrm{i}k_0 v_p(k_0)\,t}}{Z_1}\,\mathcal{N}\left(x \mid c_1 + v_g(k_0)\,t, \sigma^2 + \mathrm{i}\,t\,\mathcal{H}(k_0)\right)\mathrm{e}^{\mathrm{i}k_0 x}\,,\\
\Psi_2(x,t) &= \frac{\mathrm{e}^{-\mathrm{i}k_0 v_p(k_0)\,t}}{Z_1}\,\mathcal{N}\left(x \mid c_2 - v_g(k_0)\,t, \sigma^2 + \mathrm{i}\,t\,\mathcal{H}(-k_0)\right)\mathrm{e}^{-\mathrm{i}k_0 x}\,,\\
\Phi_1(k,t) &= \frac{\mathrm{e}^{-\mathrm{i}t\,v_p(k_0)k_0}}{Z_{k_0}}\,\mathcal{N}\left(k \mid k_0, (\sigma^2 + \mathrm{i}\,t\,\mathcal{H}(k_0))^{-1}\right)\,\mathrm{e}^{\mathrm{i}(k-k_0)\left(c_1+v_g(k_0)\,t\right)}\,,\\
\Phi_2(k,t) &= \frac{\mathrm{e}^{-\mathrm{i}t\,v_p(k_0)k_0}}{Z_{k_0}}\,\mathcal{N}\left(k \mid -k_0, (\sigma^2 + \mathrm{i}\,t\,\mathcal{H}(-k_0))^{-1}\right)\,\mathrm{e}^{\mathrm{i}(k+k_0)\left(c_2-v_g(k_0)\,t\right)}\,. \qquad (3)
\end{aligned}$$

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.

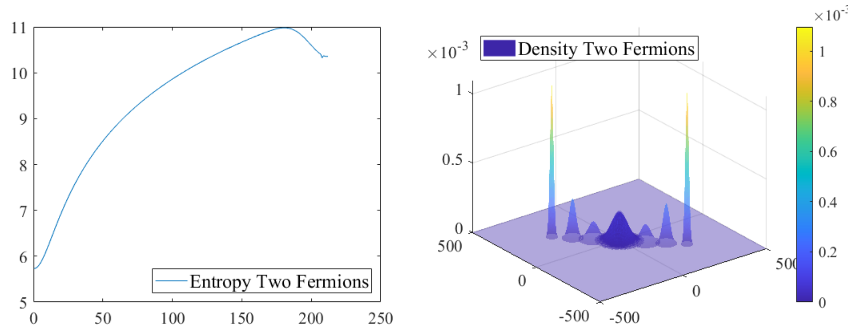
The Hydrogen Atom and Photon Emission

The QED Hamiltonian for the hydrogen atom is

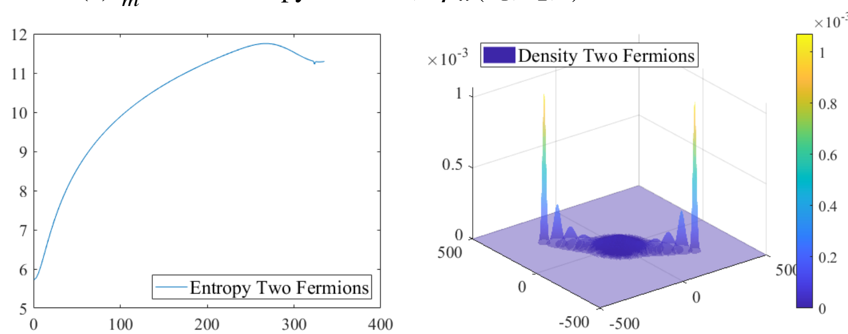
$$H(p,r,q) = \sum_{i=1}^{3}\frac{\left(p^i - \frac{\mathrm{e}}{c}A^i(q)\right)^2}{2m} - \frac{\mathrm{e}^2}{r} + \sum_{\lambda=1}^{2}\hbar\omega_q\,a_\lambda^\dagger(q)\,a_\lambda(q)\,,$$

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 $A = (A^1, A^2, A^3)$. 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 (3), 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 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 $\Delta E_{n=2\to n=1} \approx -\left(\frac{1}{2^2}-1\right) \times 13.6\,\mathrm{eV} = 10.2\,\mathrm{eV}$. We now compute the difference between the final and initial state entropy following three steps.

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

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

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

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

$$-0.740\,.$$

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 occur in nature, 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 $K^0 \mapsto \bar{K}^0$ to create an antiparticle's QCurve e_1 in $\mathcal{I}$.

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

CONCLUSIONS

Capturing all the information of a quantum state requires the specifying of the parameters associated to the DOFs of a quantum state as well as as the intrinsic randomness of the quantum state. We proposed an entropy defined in the phase spaces of position and spatial frequency as well as in the spin phase space addressing the space and the spin DOFs. This definition of the entropy possesses desirable properties, including invariance in special relativity, and invariance under CPT transformations.

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 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 particle states with QCurves in $\mathcal{O}$ to transform into new states with the creation and annihilation of particles.

---

[1] W. Beckner. *Inequalities in Fourier analysis.* PhD thesis, Princeton., 1975.

[2] I. Białynicki-Birula and J. Mycielski. Uncertainty relations for information entropy in wave mechanics. *Commun. Math. Phys.*, 44(2):129–132, 1975.

[3] B. H. Bransden and C. J. Joachain. *Physics of atoms and molecules*. Addison-Wesley, 2003.

[4] J. H. Christenson, J. W. Cronin, V. L. Fitch, and R. Turlay. Evidence for the 2π decay of the K_2^0 meson. *Phys. Rev. Lett.*, 13:138–140, Jul 1964.

[5] R. Clausius. *The mechanical theory of heat: With its applications to the steam-engine and to the physical properties of bodies*. J. van Voorst, 1867.

[6] C. Cohen-Tannoudji, B. Diu, and F. Laloe. *Quantum Mechanics: Volume 1, Basic concepts, tool, and applications*. Wiley-VCH, 2 edition, 2019.

[7] A. Dembo, T. M. Cover, and J. A. Thomas. Information theoretic inequalities. *IEEE Transactions on Information Theory*, 37(6):1501–1518, 1991.

[8] P. A. M. Dirac. The quantum theory of the emission and absorption of radiation. *Proc. R. Soc. Lond. A*, 114:243–265, 1927.

[9] E. Fermi. *Nuclear physics: A course given by Enrico Fermi at the University of Chicago*. University of Chicago Press, 1950.

[10] R. P. Feynman and S. Weinberg, editors. *Elementary particles and the laws of physics: The 1986 Dirac memorial lectures*. Cambridge University Press, 1999.

[11] D. Geiger and Z. M. Kedem. Quantum information physics II. New York University, Dept. of Computer Science,TR 2021-997, 2021.

[12] W. Gerlach and O. Stern. Der experimentelle Nachweis des magnetischen Moments des Silberatoms. *Z. Phys.*, 8(1):110–111, 1922.

[13] J. W. Gibbs. *Elementary principles in statistical mechanics*. Courier Corporation, 2014.

[14] I. I. Hirschman. A note on entropy. *Am. J. Math.*, 79(1):152–156, 1957.

[15] E. T. Jaynes. Gibbs vs Boltzmann entropies. *Am. J. Phys.*, 33(5):391–398, 1965.

[16] H. P. Robertson. The uncertainty principle. *Physical Review*, 34:163–164, Jul 1929.

[17] J. J. Sakurai. *Modern Quantum Mechanics*. Cambridge University Press, 2 edition, 2017.

[18] J. von Neumann. *Mathematical foundations of quantum mechanics: New edition*. Princeton University Press, 2018.

[19] S. Weinberg. *The quantum theory of fields: Volume 1, (Foundations)*. Cambridge University Press, 1995.