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# $H$-theorem in quantum physics

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## ABSTRACT

Remarkable progress of quantum information theory (QIT) allowed to formulate mathematical theorems for conditions that data-transmitting or data-processing occurs with a non-negative entropy gain. However, relation of these results formulated in terms of entropy gain in quantum channels to temporal evolution of real physical systems is not thoroughly understood. Here we build on the mathematical formalism provided by QIT to formulate the quantum $H$-theorem in terms of physical observables. We discuss the manifestation of the second law of thermodynamics in quantum physics and uncover special situations where the second law can be violated. We further demonstrate that the typical evolution of energy-isolated quantum systems occurs with non-diminishing entropy.

## Introduction

Boltzmann's foundational $H$-theorem[1,2] states that evolution of systems described by a distribution function obeying the kinetic equation occurs with non-diminishing entropy. Defining entropy through the quantum mechanical density matrix $\hat{\rho}$ as $S(\hat{\rho}) = -k_{\rm B}\mathrm{tr}\{\hat{\rho}\log\hat{\rho}\}$, von Neumann conjectured[3] a solely quantum origin of the $H$-theorem. A decades-long pursuit of the proof of this key conjecture[4] was crowned by recent progress in quantum information theory (QIT), which formulated several rigorous mathematical theorems about the conditions for a non-negative entropy gain[5,6].

To describe quantum dynamics of an open system, the quantum information theory introduces the so-called *quantum channel* (QC) defined as a trace-preserving completely positive map, $\hat{\tilde{\rho}} = \Phi(\hat{\rho})$, of a density matrix[5]. The entropy gain in a channel $\Phi(\hat{\rho})$ is[7]

$$S(\Phi(\hat{\rho})) - S(\hat{\rho}) \geqslant -k_{\rm B}\mathrm{tr}\{\Phi(\hat{\rho})\log\Phi(\hat{1})\}, \tag{1}$$

where $\hat{1}$ is the unit matrix. The most general class of the channels for which the entropy gain $\Delta S \equiv S(\hat{\tilde{\rho}}) - S(\hat{\rho}) \geqslant 0$, is the so-called *unital* channel defined by the relation[5,6] $\Phi(\hat{1}) = \hat{1}$, so that $\mathrm{tr}\{\Phi(\hat{\rho})\log\Phi(\hat{1})\} = 0$. Then within the framework of the QIT one can formulate the quantum $H$-theorem as follows: the entropy gain during evolution is nonnegative if and only if the system evolution can be described by the unital channel. (Indeed, one can show that for a quantum system endowed with the finite $N$-dimensional Hilbert space, the unitality condition becomes not only a sufficient, but also the necessary condition for non-diminishing entropy. The unitality of the channel imply that non-diminishing entropy, $\Delta S \geqslant 0$, arises for *any* initial state of the system. If the channel is not unital, then there exist states, for which $\Delta S < 0$. E.g. this is correct for the chaotic state where $\rho = I/N$ (for finite dimension, $N$, case). For an infinite-dimensional quantum system the entropy is not continuous[8], and this situation requires special consideration. Finally, it is noteworthy that there exist certain classes of states that evolve with $\Delta S \geqslant 0$ even if the channel is not unital[9].) To connect this formulation to the realm of physics note that any quantum system interacting with the reservoir generates a quantum channel. Indeed, let us consider joint evolution of the grand system, comprising a given quantum system and a reservoir initially prepared in a disentangled state, $\hat{\mathscr{P}} = \hat{\rho}\otimes\hat{\rho}_{\rm R}$, where $\hat{\rho}_{\rm R}$ is the density matrix of the reservoir. (The evolution from an initially entangled state may be accompanied by the arbitrary gain in entropy. This demonstrates the necessity of the disentanglement condition. Examples of how the initially entangled system can evolve with the decreasing entropy are given e.g. in Refs. 10, 11.) Let $\hat{U}$ be the unitary operator describing the temporal evolution of the grand system. Then, according to the Stinespring-Kraus dilation theorem[5] $\Phi(\hat{\rho}) = \mathrm{tr}_{\rm R}\{\hat{U}\hat{\mathscr{P}}\hat{U}^{\dagger}\}$ is the quantum channel.

## Quantum $H$-theorem

In physics the positive entropy gain, according to the second law of thermodynamics, is ensured by the energy isolation of the evolving system, see detailed discussion in Supplementary Information (SI). Accordingly, in what follows we discuss the

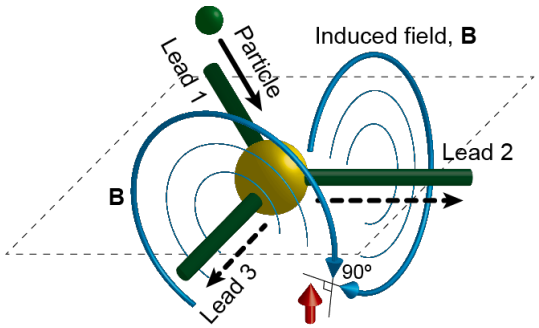


**Figure 1.** Scattering in a 3-lead setup. A particle incident from the lead 1 is scattered into two other leads 2 and 3. Propagating particle induces magnetic field perpendicular to the lead direction. The spin is placed at the point where the respective fields induced by particles propagating along leads 2 and 3 are perpendicular to each other. To simplify consideration, we choose the set up design allowing to neglect the field induced by the particle in the lead 1.

systems energy-isolated from the reservoir. Furthermore, we will be assuming that our systems are initially disentangled from the reservoir. Let us consider a fixed energy subspace $E$ of the system Hilbert space spanned by the orthonormal basis states $|\psi_{i,E}\rangle$, where index $i$ denotes all the remaining system's degrees of freedom. It is convenient to present the evolution operator, $\hat{U}$, of the grand system (a system plus reservoir) as

$$\hat{U} = \sum\nolimits_E |\psi_{j,E}\rangle\langle\psi_{i,E}| s_{ji,E}\hat{F}_{ji,E}, \tag{2}$$

The factorization into $s_{ji,E}$ and $\hat{F}_{ji,E}$ is not unique, so we will be choosing the most suitable one for each particular case. For example, considering below a particle interacting with a spin, we will let $s_{ji,E}$ be the components of the scattering matrix corresponding to the transition amplitude between the particle states $|\psi_{i,E}\rangle \to |\psi_{j,E}\rangle$ (without taking into account interaction with the spin).

Operators $\hat{F}_{ji,E}$ are the family of operators acting in the reservoir Hilbert space, where subscripts $i$, $j$, and $E$ specify the particle state. For an energy-isolated quantum system the quantum states at different energies transform independently. To determine whether the evolution belongs in the class of the unitality channel, one has to check if the system obeys the $\Phi(\hat{1}) = \hat{1}$ relation. Using the unitarity of $\hat{U}$, one finds (see SI 1 and SI 2)

$$\Phi_{jj'}(\hat{1}_E) = [\hat{1}_E]_{jj'} + \sum\nolimits_i s_{ji,E} s^*_{j'i,E} \langle [\hat{F}^\dagger_{j'i}, \hat{F}_{ji}]\rangle, \tag{3}$$

where $\langle\ldots\rangle$ is averaging with respect to the initial state of the reservoir, and $\hat{1}_E = \sum_i |\psi_{j,E}\rangle\langle\psi_{i,E}|$. This relation is our central result. It establishes the criterion for unitality of the energy-isolated system in terms of physical operators describing the interaction of the quantum system with the reservoir and allows to formulate quantum $H$-theorem as follows.

*Let the quantum system interacting with the reservoir be initially disentangled from it and be energy-isolated during the evolution. Let* $\sum_i s_{ji,E} s^*_{j'i,E} \langle [\hat{F}^\dagger_{j'i}, \hat{F}_{ji}]\rangle = 0$*, where operators* $\hat{F}_{ji,E}$ *and coefficients* $s_{ji,E}$ *are defined as in Eq. (2), for energies* $E$ *at which the system can be found with finite probability, i.e. for energies such that* $\langle\psi_{j,E}|\,\hat{\rho}\,|\psi_{j,E}\rangle \neq 0$*. Then the entropy gain* $\Delta S = S(\Phi(\hat{\rho})) - S(\hat{\rho}) \geqslant 0$*.*

The obtained formulation of the quantum $H$-theorem enables us to reveal a fundamental difference in how the second law of thermodynamics manifests itself in quantum and classical physics. In classical thermodynamics the energy-isolated system inevitably evolves with non-diminishing entropy. We find that in quantum physics it is different. To demonstrate that, we construct an energy-isolated quantum system for which $\langle [\hat{F}^\dagger_{j'i}, \hat{F}_{ji}]\rangle \neq 0$ and which thus evolves with the negative entropy gain. Let us consider a charged particle moving in a three-lead conductor and interacting with the spin via the induced magnetic field, see Fig. 1, and, according to our general framework, initially disentangled from the spin. In the absence of the external magnetic field the energy exchange is absent and the particle is energy-isolated. The joint scattering states of the particle and spin have the form

$$|\psi^{(\mathrm{in})}_\alpha\rangle|\sigma_0\rangle \to \sum\nolimits_\beta s_{\beta\alpha}\,|\psi^{(\mathrm{out})}_\beta\rangle\,\hat{U}_\beta\hat{U}^\dagger_\alpha|\sigma_0\rangle, \tag{4}$$

where $|\psi^{(\mathrm{in/out})}_\alpha\rangle$ is the particle's incoming/outgoing state in the lead $\alpha$, $s_{\beta\alpha}$ are the components of the scattering matrix of the three lead set up, $|\sigma_0\rangle$ is the initial state of the spin and $\hat{U}_\alpha$ ($\hat{U}^\dagger_\alpha$) is the unitary spin-1/2 rotation of the spin due to outgoing (incoming) electron in the lead $\alpha$. Then the operators $\hat{F}$ of Eq. (3) are defined as $\hat{F}_{\beta\alpha} = \hat{U}_\beta\hat{U}^\dagger_\alpha$.

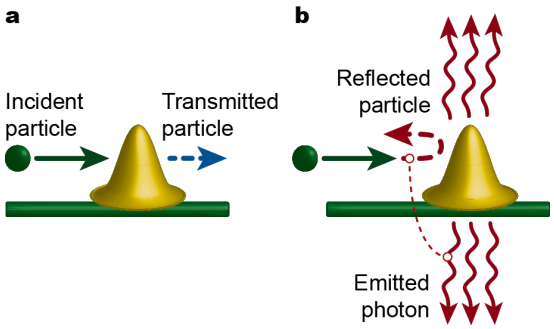


**Figure 2.** Braking radiation in 1D. a. A scattering where electron is transmitted without photon emission. b. A backward scattering event accompanied by the emission of photons.

Let us recall now that rotations of a spin about different axis in general do not commute. We choose spin-$1/2$ rotations as $\hat{U}_1 = \hat{1}$, $\hat{U}_2 = i\hat{\sigma}_x$ and $\hat{U}_3 = i\hat{\sigma}_y$, where $\hat{\sigma}_x$ and $\hat{\sigma}_y$ are the Pauli matrices, so that $[\hat{U}_\alpha, \hat{U}_\beta] \neq 0$. Accordingly, $\langle [\hat{F}^\dagger_{\beta'\alpha}, \hat{F}_{\beta\alpha}] \rangle \neq 0$, and the resulting quantum channel is non-unital. The explicit calculation gives (see SI 3)

$$\Phi(\hat{1}_E) = \hat{1}_E + 2i\left\{ |1\rangle\langle 2|\, s_{13,E} s^*_{23,E}\, \langle\hat{\sigma}_x\rangle \right. \\ \left. + |1\rangle\langle 3|\, s_{12,E} s^*_{23,E}\, \langle\hat{\sigma}_y\rangle - |2\rangle\langle 3|\, s_{12,E} s^*_{13,E}\, \langle\hat{\sigma}_z\rangle - \text{H.c.} \right\}. \tag{5}$$

Let the initial state of the spin be a pure state $|S_0\rangle = (|\uparrow_x\rangle + |\uparrow_y\rangle + |\uparrow_z\rangle)/\sqrt{3}$, so that all the $\langle\hat{\sigma}_\alpha\rangle$ in the Eq. (5) are equal to $1/3$. Hence all off-diagonal elements of $\Phi(\hat{1}_E)$ appear finite. Taking all $s = 2/3$, at some energy $E_0$, we construct the normalized initial state of the particle as $\hat{\rho} = (1/6)\int dE\, f(E - E_0)\hat{1}_E$, with $f(E)$ being the normalized to unity distribution function centered around $E = 0$ and rapidly decaying as $|E| \to \infty$, and obtain $\Delta S \approx -0.05\, k_B$. We thus demonstrated that even the energy isolation does not guarantee the evolution with the non-diminishing entropy. Note that in the discussed example the reservoir acts as some quantum analogue of the classical Maxwell demon. Namely, having been prepared in a special state, the reservoir is able to decrease the entropy of the system without the energy exchange with it, and can be referred to as a 'quantum Maxwell demon.' The applications of the quantum Maxwell demon concept for making quantum thermal machines will be published elsewhere.

## Elastic scattering

As a first example of a system satisfying quantum $H$-theorem, we consider an electron elastically scattered by the one-dimensional (1D) potential barrier, see Fig. 2. Let the electron reflection be accompanied by the change of the reservoir state (e.g. let the reflection to imply emission of the low energy photon via braking radiation, or scattering of the photon), see Fig. 2b, and the electron transmission to retain the state of the reservoir, see Fig. 2a. Accordingly, the joint scattering states of the particle with the fixed energy assume the form,

$$|\mathrm{L}\rangle|n\rangle \to s_{\mathrm{RL}}|\mathrm{R}\rangle|n\rangle + s_{\mathrm{LL}}|\mathrm{L}\rangle|n'\rangle, \tag{6}$$

$$|\mathrm{R}\rangle|n\rangle \to s_{\mathrm{LR}}|\mathrm{L}\rangle|n\rangle + s_{\mathrm{RR}}|\mathrm{R}\rangle|n''\rangle, \tag{7}$$

where indices $\{\mathrm{L},\mathrm{R}\}$ denote the incident (scattered) states in the left and right leads, respectively, $|n\rangle$ is the initial reservoir state, and $|n'\rangle$ and $|n''\rangle$ are the reservoir states resulting from the backscattering to the left and to the right, respectively. The unitality of the corresponding channel follows now from general Eq. (3), see SI 4. However, for illustrative purpose we derive unitality straightforwardly using the explicit form of Eq. (6) and Eq. (7). Namely, calculating $\hat{1}_E$ in the basis of left and right scattering channels, $i, j \in \{\mathrm{L},\mathrm{R}\}$, we obtain

$$\hat{1}_E \to |\mathrm{R}\rangle\langle\mathrm{R}|\,(|s_{\mathrm{RR}}|^2 + |s_{\mathrm{RL}}|^2) + |\mathrm{L}\rangle\langle\mathrm{L}|\,(|s_{\mathrm{LR}}|^2 + |s_{\mathrm{LL}}|^2) + \\ \left\{ |\mathrm{R}\rangle\langle\mathrm{L}|\,(s^*_{\mathrm{LR}} s_{\mathrm{RR}}\langle n''|n\rangle + s^*_{\mathrm{LL}} s_{\mathrm{RL}}\langle n|n''\rangle) + \text{H.c.} \right\} \tag{8}$$

and taking into account the unitarity of the overall transformation, we arrive at $\Phi(\hat{1}_E) = \hat{1}_E$. Since this condition holds for any $E$, then for any state the system evolves with $\Delta S \geqslant 0$. The above consideration with some minor modifications holds for the grand system where the role of the reservoir is taken up by a single spin located near the scatterer. Then the spin remains intact if the particle is reflected and is rotated by the magnetic field induced by the transmitted particle.

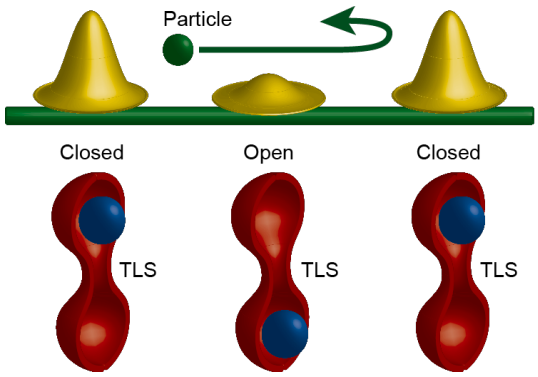


**Figure 3.** 1D random walk of an electron. Two-level systems (TLSs) shown as double well potentials are located equidistantly along the wire. Each TLS forms an effective potential for the electron, which depends on the TLS's quantum state. For simplicity we consider a completely transparent (open) or completely reflective (closed) effective scattering potential depending on the TLS state. At each scattering event the set of TLSs is replaced by a new (unentangled) one.

Let us generalize the above consideration onto the particle propagating along the two-dimensional array of scatterers and spins (comprising the reservoir) located in the $xy$-plane. The magnetic field induced by the propagating particle is perpendicular to the plane, and all spins experience the commuting unitary rotations around the perpendicular $z$-axis. All the rotations commute, hence the condition of the quantum $H$-theorem is satisfied and $\Delta S \geqslant 0$.

Remarkably, the property of unitality of the grand system with the spin reservoir preserves in the 3D case. As we mentioned above, the rotations experienced by an individual spin may appear, in general, non-commuting. Note, however, that operators $\hat{F}$ in Eq. (3) acquire the form

$$\hat{F}_{ji} = \hat{U}_{ji}^{(1)} \otimes \ldots \otimes \hat{U}_{ji}^{(N)}, \tag{9}$$

where $\hat{U}_{ji}^{(a)}$ is a unitary rotation of a spin $a$ by the electron experienced a scattering process from the state $|i\rangle$ to the state $|j\rangle$. Then

$$[\hat{F}_{j'i}^{\dagger}, \hat{F}_{ji}] = \prod_{a=1}^{N} \otimes \hat{U}_{j'i}^{\dagger(a)} \hat{U}_{ji}^{(a)} - \prod_{a=1}^{N} \otimes \hat{U}_{ji}^{(1)} \hat{U}_{j'i}^{\dagger(1)}, \tag{10}$$

where $N \gg 1$ is the total number of spins. For most of the spins, the factors that appear upon averaging Eq. (10) are small, $\langle \hat{U}_{j'i}^{\dagger(a)} \hat{U}_{ji}^{(a)} \rangle$, $\langle \hat{U}_{ji}^{(a)} \hat{U}_{j'i}^{\dagger(a)} \rangle < q < 1$. Therefore, we arrive at the estimate

$$\langle [\hat{F}_{j'i}^{\dagger}, \hat{F}_{ji}] \rangle \lesssim \exp[-N \ln(1/q)], \tag{11}$$

therefore, $\langle [\hat{F}_{j'i}^{\dagger}, \hat{F}_{ji}] \rangle \to 0$ as $N \to \infty$. We see that in the macroscopic limit of the number of spins, the averaged commutators appearing in the condition for the $H$-theorem vanish in spite of the fact that the commutators for the individual spins could remain finite. Thus the evolution of the 3D system involved occurs with $\Delta S \geqslant 0$.

To proceed further, we note, that if one can find a basis in the reservoir Hilbert space where all $\hat{F}_{ji}$-operators are diagonal, then the operators $\hat{F}_{ji}$ commute. Below we present two generic physical examples where this basis can be found explicitly: (i) an electron interacting with adiabatic two-level impurities and (ii) electron-phonon interaction in solids.

## Scattering on two-level systems

Consider the electron scattering on impurities that fluctuate between two positions with nearly equal energies. To be concrete we focus on the random walk of the electron along the ensemble of TLS (see the description of the similar systems in Refs. 12, 13) as shown in Fig. 3. Assume for simplicity that (i) the dynamics of a TLS is slow hence its state does not change during the interaction with the electron and that (ii) each TLS which is in the state $|\uparrow\rangle$ ($|\downarrow\rangle$), scatters the electron via elastic unitary matrix $\hat{S}_{\uparrow}$ ($\hat{S}_{\downarrow}$). Then the global unitary transformation is given by $\hat{U} = \prod_n \otimes \hat{U}_n$ where $\hat{U}_n = \hat{S}_{\uparrow}^{(n)} |\uparrow_n\rangle\langle\uparrow_n| + \hat{S}_{\downarrow}^{(n)} |\downarrow_n\rangle\langle\downarrow_n|$ describes the scattering on the $n$-th impurity. Denote the scattering state of the electron moving in a direction $\mathbf{k}$ by $|\mathbf{k}\rangle$. Then the reservoir operator $\hat{F}_{\mathbf{k}\mathbf{k}'} = \prod_n \otimes \hat{F}_{\mathbf{k}\mathbf{k}'}^{(n)}$ with $\hat{F}_{\mathbf{k}\mathbf{k}'}^{(n)} = [\hat{S}_{\uparrow}^{(n)}]_{\mathbf{k}\mathbf{k}'} |\uparrow_n\rangle\langle\uparrow_n| + [\hat{S}_{\downarrow}^{(n)}]_{\mathbf{k}\mathbf{k}'} |\downarrow_n\rangle\langle\downarrow_n|$, see Eq. (2), commute with each other and, therefore, the second term in Eq. (3) vanishes. Hence, in each particular scattering event the entropy of the particle is non-diminishing.

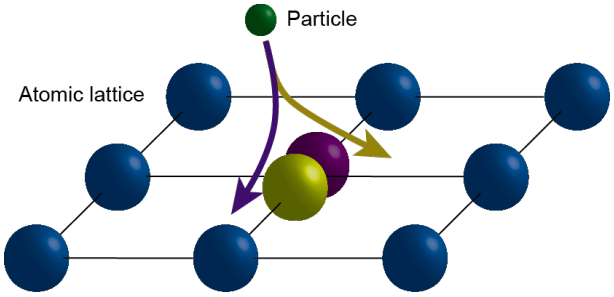


**Figure 4.** Electrons and phonons in an atomic lattice. The scattering state of an electron depends strongly on the position of the scattering atom in the lattice. Importantly, the position of the scatterer remains almost unchanged during the scattering process because of the significant mass difference between the scattered electron and the scattering atom.

The question that now arises is whether the non-diminishing entropy maintains for the sequence of scatterings. Recall that in order for the entropy to grow monotonously, an electron should be disentangled from the TLS with which it is going to interact. Since in the course of the evolution an electron may return to the TLS on which it scattered and, therefore, got entangled in the past, these returns would violate this 'initial non-entanglement condition.' Thus to guarantee the evolution with non-diminishing entropy the TLS should have interacted with some other degrees of freedom that would lead to the memory loss of this TLS prior to the possible return of the electron. This memory loss is the manifestation of the so-called *monogamy* of entanglement[14] which is a specific property of the entanglement distribution between quantum systems: if a TLS is already entangled with an electron and later it becomes entangled with another degree of freedom then the initial entanglement with the electron vanishes. Thus the process of sequential scattering of an electron satisfies the $H$-theorem if the typical entanglement time for the TLS is less than the typical return time of an electron to particular TLS.

## Electron-phonon interaction

Now we demonstrate that the electron-phonon interaction leads to the electron evolution which satisfies the conditions of quantum $H$-theorem. In a standard electron-phonon interaction model, a representative test electron 'sees' a screened short-range ionic potential. Since the resulting scattering time is short and the ion is much heavier than the electron, the position of a given ion remains nearly unchanged during the interaction with the electron, see Fig. 4. Then the standard consideration of the electron-phonon interaction[15] results in a conclusion that at high temperatures where the typical energy of an electron is relatively high (i.e. it exceeds the Debye energy, the maximal energy of phonons), the electron-phonon collisions are quasi-elastic. This allows us to apply the same arguments as for the model of an electron interacting with two-level impurities considered above. Indeed, the slow ion-dynamics preserves the classical distribution function, $\rho_{\rm ion}(\{\mathbf{r}\})$, for the ions positions $\{\mathbf{r}\}=\{\mathbf{r}_1,\mathbf{r}_2,\ldots\}$ and hence the induced $\hat{F}$-operators are diagonal in the ion coordinate basis, $\hat{F}_{ji}=\int\prod_\alpha d\mathbf{r}_\alpha\, s_{ji}(\{\mathbf{r}\})\rho_{\rm ion}(\{\mathbf{r}\})\prod_\alpha|\mathbf{r}_\alpha\rangle\langle\mathbf{r}_\alpha|$, where $s_{ji}(\{\mathbf{r}\})$ are electron scattering matrix on the potential defined by the ions positions $\{\mathbf{r}\}$. Therefore the conditions of the quantum $H$-theorem hold for electrons with energies exceeding the Debye energy. The initial disentanglement of the electron from the ionic reservoir is ensured either by the fact that a given ion did not participate in the previous collisions with the electron, or has already 'forgotten' about such an event due to the monogamy of entanglement.

It is noteworthy that unlike the other systems discussed in previous sections, the evolution of the electron-phonon system does not occur in the unital channel. Nevertheless, it satisfies the condition of the $H$-theorem thus illustrating a mathematical result establishing that for some classes of initial states even the evolution defined by non-unital channels may occur with the non-diminishing entropy[9].

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## Author contributions statement

All authors have contributed to essential portions of this work. The original idea was due to G. L.; the work was conceived by G. L. and V. V.; I. S. performed numerical simulations. All authors carried out analytical calculations, discussed the results, and contributed to the writing of the manuscript.

## Competing financial interests

The authors declare that they have no competing financial interests.