MICROSCOPIC ENTROPY AND NONLOCALITY

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We have obtained a microscopic expression for entropy in terms of $\mathcal{H}$ function based on nonunitary Λ transformation which leads from the time evolution as a unitary group to a Markovian dynamics and unifies the reversible and irreversible aspects of quantum mechanics. This requires a new representation outside the Hilbert space. In terms of $\mathcal{H}$, we show the entropy production and the entropy flow during the emission and absorption of radiation by an atom. Analyzing the time inversion experiment, we emphasize the importance of pre- and postcollisional correlations, which break the symmetry between incoming and outgoing waves. We consider the angle dependence of the $\mathcal{H}$ function in three-dimensional situation. A model including virtual transitions is discussed in a subsequent paper.

INTRODUCTION

Irreversibility in macroscopic physics is associated with entropy increase. The usual formulation of dynamics (classical or quantum) does not include irreversible processes. We have shown that this contradiction comes from the limitation to integrable systems. For a class of nonintegrable systems, dynamics includes irreversibility. For integrable systems there exists a unitary transformation U, which is distributive:

$$U(ab) = (Ua)(Ub). \tag{1}$$

For a class of nonintegrable systems (due to Poincaré resonances), we have introduced a «star unitary» invertible operator Λ which includes irreversibility and stochasticity [1–3]. This leads to a deep change in the formulation of dynamics, as it forces us to go outside the Hilbert space. Our Λ is not distributive:

$$\Lambda(ab) \neq (\Lambda a)(\Lambda b). \tag{2}$$

We have shown that there exists then an $\mathcal{H}$ function (or Lyapounov variable) [4–8] represented by the operator

$$\mathcal{H} = \Lambda^\dagger \Lambda. \tag{3}$$

Using Λ we go from the time evolution as a unitary group to a Markovian dynamics. Note also that Λ is a nonlocal transformation replacing points by ensembles. In our early work on the interaction of an atom with a field (e. g., the Friedrichs model) [9] we have shown that (3) reduces to the operator outside the Hilbert space introduced in [2, 7, 10]

$$\mathcal{H} = |\tilde{\phi}_1\rangle\langle\tilde{\phi}_1|, \tag{4}$$

where $|\tilde{\phi}_1\rangle$ is the eigenstate of the Hamiltonian H outside the Hilbert space [10, 11] with complex eigenvalue [10, 12]

$$H|\tilde{\phi}_1\rangle = z_1^{\mathrm{c.c}}|\tilde{\phi}_1\rangle, \quad z_1 = \tilde{\omega}_1 - i\gamma, \quad \tilde{\omega}_1,\, \gamma > 0, \tag{5}$$

where c. c. denotes complex conjugate. This eigenstate is called the Gamow vector [11, 12] and for the Friedrichs model, which we use in our paper, $|\tilde{\phi}_1\rangle$ is given by (9). Hence, in agreement with [1, 2, 7, 13], $\mathcal{H}$ function is an operator outside the Hilbert space with the Heisenberg evolution given by

$$\mathcal{H}(t) = \mathrm{e}^{iHt}\mathcal{H}\,\mathrm{e}^{-iHt} = \mathrm{e}^{-2\gamma t}\mathcal{H}. \tag{6}$$

The physical meaning of $\mathcal{H}$ is very simple. The expectation value of $\mathcal{H}$ decreases (and entropy increases) as the energy of the excited state is transferred to the field modes.

We make a remark here that there have always been two points of view on entropy: the point of view of Planck, relating entropy to dynamics, and the point of view of Boltzmann, relating entropy to probabilities (ignorance) [14]. We understand now that Planck could not realize his program as he worked in the usual representation of dynamics, equivalent to the Hilbert space representation.

We have now a «microscopic» formulation of thermodynamics which includes the decay and excitation of quantum states. The entropy creation is due to a resonance in the time evolution of $|\tilde{\phi}_1\rangle$. A one-dimensional situation was considered [3, 9] where an initially localized wave packet of the field interacts with an excitable particle. An essential element is the consideration of correlations. Due to the nonlocal nature of $\mathcal{H}$ function we can introduce pre- and postcollisional correlations between the particle and the field. They exist even if the wave packet corresponding to the field is at large distance from the particle. We show that the time inversion after the collision requires instant extraction of large amount of entropy from the system because the entropy after the collision is much higher than before. It means that, in order for the collision to take place, we have to create a state with a high order as we have to target our wave packet to the atom. Analyzing the scattering process we show that the second law of thermodynamics is valid as the excitation of the particle is associated with the flow of entropy that is provided by the incoming wave packet [9]. The amount of entropy provided decides the amount of excitation of the ground state. This will be further discussed in subsequent papers. The interest of these considerations is to introduce space dependence in the thermodynamic evolution.

These effects were extended to the three-dimensional problem where the direction of the initial momentum of the wave packet and the possibility for the wave packet to be scattered in all direction of the three-dimensional space results in more complicated picture.

1. $\mathcal{H}$ FUNCTION IN THE FRIEDRICHS MODEL

The Friedrichs model for the interaction of matter with radiation in the rotating wave approximation is given by the Hamiltonian (with units $\hbar = c = 1$)[1]

$$H = \omega_1|1\rangle\langle 1| + \sum_k \omega_k|k\rangle\langle k| + \lambda\sum_k V_k\left(|1\rangle\langle k| + |k\rangle\langle 1|\right), \tag{7}$$

[1] We shall extend this consideration including virtual transitions in subsequent papers.

where $|1\rangle$ represents a bare particle or atom in its excited state with no photons present, while the state $|k\rangle$ represents a bare field mode of the momentum k and the particle in its ground state. The momentum in the volume L is quantized $k = (2\pi)^d n/L$; n is integer vector with the space with the dimension d. The energy of the ground state is chosen to be zero; ω_1 is the bare energy of the excited level, and $\omega_k \equiv |k|$ is the photon energy. The coupling constant λ is dimensionless. For $\alpha, \beta = 1, k$ we have orthonormality and completeness relations $\langle\alpha|\beta\rangle = \delta_{\alpha,\beta}$, $\sum_{\alpha=1,k} |\alpha\rangle\langle\alpha| = 1$. In the infinite volume limit $L \to \infty$, the momentum k becomes continuous, i.e.,

$$\sum_k \to \frac{L}{(2\pi)^d} \int d^d k, \quad V_k = \frac{(2\pi)^{d/2}}{L^{d/2}} v_k\,, \quad v_k \sim L^0, \tag{8}$$

where the integration is taken over «d» dimensional k space. When $\omega_1 > \int dk \lambda^2 v_k^2/\omega_k$ the excited state is unstable due to resonance between the particle and the field. In this case, the Gamow vector $|\tilde{\phi}_1\rangle$ is [10, 12]

$$|\tilde{\phi}_1\rangle = N_1^{1/2} \left[|1\rangle + \sum_k \frac{\lambda V_k}{[\omega_k - z_1^{\rm c.c}]_-} |k\rangle \right], \tag{9}$$

where N_1 is a normalization constant and the distribution $1/[\omega_k - z_1^{\rm c.c}]_-$ is defined with the help of suitable test function $\varphi(\omega_k)$ as

$$\int dk \frac{\varphi(\omega_k)}{[\omega_k - z_1^{\rm c.c}]_-} \equiv \int dk \frac{\varphi(\omega_k)}{\omega_k - z_1} - 2\pi i \varphi(z_1^{\rm c.c}). \tag{10}$$

Note that the transition from the bare state to the Gamow vector is «star unitary» (see [10]). We shall consider the $\mathcal{H}_\xi(t)$ function defined as the expectation value of the $\mathcal{H}$ operator:

$$\mathcal{H}_\xi(t) \equiv \langle\xi|{\rm e}^{iHt}\mathcal{H}\,{\rm e}^{-iHt}|\xi\rangle, \tag{11}$$

where the initial state $|\xi\rangle$ corresponds to the particle located at $x = 0$ in its ground state and a localized wave packet formed by the field.

2. MOMENTUM INVERSION EXPERIMENT

We consider the momentum inversion experiment [9, 10] with the wave packet initially localized in a finite interval of size a:

$$\langle x|\xi\rangle = \frac{{\rm e}^{ik_0 x}}{W^{1/2}} \theta\left(\frac{a}{2} - |x - x_0|\right), \quad \langle k|\xi\rangle = -\frac{2\omega_k}{W}\,{\rm e}^{-i(k-k_0)x_0} \frac{\sin\left[a(k-k_0)/2\right]}{k - k_0}. \tag{12}$$

The wave packet is centered at x_0, and an initial momentum $k_0 > 0$ is directed to the particle.

We observe the time evolution of $|\xi\rangle$ determined by the Hamiltonian H and calculate $\mathcal{H}_\xi(t)$ (11) as a function of t. At some moment t_1, we perform the momentum inversion by the antilinear time-inversion operator T_I [7] that inverts the sign of time t and the momentum of the field modes. Then we observe the time evolution of the transformed state further. The results of these observations are presented in Fig. 1. We see that $\mathcal{H}_\xi(t)$ function decays exponentially with time. This corresponds to the increase of the entropy in the system in accordance with the second law of thermodynamics.

The time inversion made at time t_i introduces the instant effect of the outside world which leads to a jump of the $\mathcal{H}_\xi(t)$ function. The jump depends on the time the momentum inversion is performed:

1) The time inversion made at t_2, that is, after the collision leads to a drastic increase of $\mathcal{H}_\xi(t)$ function. The time inversion replaces the scattered outgoing field by an incoming wave targeted to the particle. This creates correlations between the particle and the field which are precollisonal correlations. This lowers the entropy. As a consequence, the expectation value of $\mathcal{H}_\xi(t)$ «jumps» to a higher value.

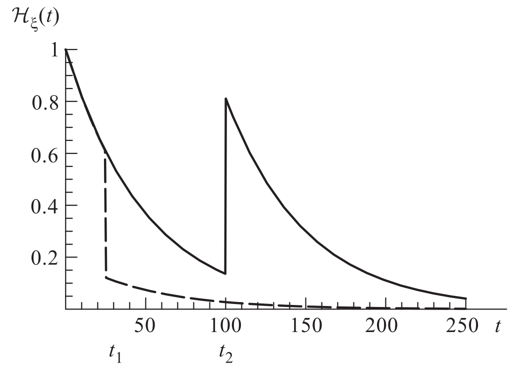

Fig. 1. The momentum inversion experiments performed at time t_1, that is, before the collision (destroys precollisional correlations) and at time t_2, that is, after the collision (replaces postcollisional correlations by the precollisional ones)

2) The inversion performed at time t_1, that is, before the collision and replaces the incoming wave by an outgoing one, which will not collide with the particle. This destroys precollisional correlations and, therefore, increases the entropy. The expectation value of $\mathcal{H}$ «jumps» to a lower value corresponding to postcollisional correlations.

The basic distinction between precollisional and postcollisional correlations takes into account the change of the entropy. As we noticed, precollisional correlations increase the $\mathcal{H}_\xi(t)$ function. This observation has already been made many years ago [1]. The emission of photons corresponds to a postcollisional correlation decreasing the $\mathcal{H}_\xi(t)$ function as photons escape from the particle. The details of the collision showing the difference between pre- and postcollisional correlations are given in the next section.

3. ENTROPY PRODUCTION AND ENTROPY FLOW DURING THE COLLISION

Using the completeness of the $|1\rangle$, $|k\rangle$ basis we can express the $\mathcal{H}_\xi$ (11) as a sum:

$$\mathcal{H}_\xi(t) = \mathcal{H}_{11}(t) + \mathcal{H}_{1f}(t) + \mathcal{H}_{ff}(t), \tag{13}$$

where

$$\mathcal{H}_{11}(t) = \left|\langle\xi|\mathrm{e}^{iHt}|1\rangle\langle 1|\tilde{\phi}_1\rangle\right|^2, \tag{14}$$

$$\mathcal{H}_{1f}(t) = \sum_k \langle\xi|\mathrm{e}^{iHt}|k\rangle\langle k|\tilde{\phi}_1\rangle\langle\tilde{\phi}_1|1\rangle\langle 1\mathrm{e}^{-iHt}|\xi\rangle + \text{c. c.}, \tag{15}$$

$$\mathcal{H}_{ff}(t) = \left|\sum_k \langle\xi|\mathrm{e}^{iHt}|k\rangle\langle k|\tilde{\phi}_1\rangle\right|^2, \tag{16}$$

where $\mathcal{H}_{11}(t)$, $\mathcal{H}_{ff}(t)$, and $\mathcal{H}_{1f}(t)$ correspond to the particle, field, and field–particle correlation. Knowing $|\tilde{\phi}_1\rangle$ (see (9)) it is elementary to evaluate the time dependence of these components. In the continuous limit using the pole approximation, we have

$$\mathcal{H}_{11}(t) \approx C\left(1 - \mathrm{e}^{-\gamma(x_1+t)}\right)^2, \tag{17}$$

$$\mathcal{H}_{1f}(t) \approx 2C(1 - \mathrm{e}^{-\gamma(x_1+t)})(\mathrm{e}^{-\gamma(x_2+t)} - 1) + \text{c. c.}, \tag{18}$$

$$\mathcal{H}_{ff}(t) \approx C(\mathrm{e}^{-\gamma(x_2+t)} - 1)^2, \tag{19}$$

where C is a constant determined by the interaction λV_k and by the initial wave packet $|\xi\rangle$.

In Fig. 2, we see that the total entropy production in the system expressed by the exponentially decreasing curve $\mathcal{H}_\xi(t)$ may be divided into three different time intervals:

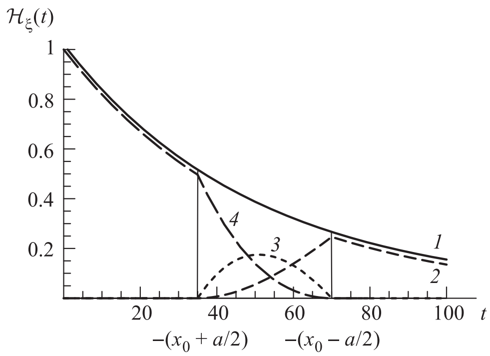

Fig. 2. Entropy production and the entropy flow during the collision: curve *1* — $\mathcal{H}_\xi(t)$; curve *2* — $\mathcal{H}_{11}(t)$; curve *3* — $\mathcal{H}_{1f}(t)$; curve *4* — $\mathcal{H}_{ff}(t)$

1) $0 < t < -(x_0 - a/2)$, before the collision. Initially, the entropy of the system is low ($\mathcal{H}_\xi(t)$ function is high) because the wave packet is «targeted» to the particle; i. e., a higher order is created in the system by «anomalous» precollisional correlations. Here, only the field part, $\mathcal{H}_{ff}$, contributes to the total entropy $\mathcal{H}_\xi(t)$ of the system as the particle is in its ground state, therefore, $\mathcal{H}_{11} = 0$. As the wave packet approaches the particle $\mathcal{H}$ decreases.

2) $-(x_0 + a/2) < t < -(x_0 - a/2)$, during the collision. The particle (curve *2*, $\mathcal{H}_{11}$) goes to its excited state with lower entropy.

3) $-(x_0 + a/2) < t$, after the collision. The excited particle contributes to $\mathcal{H}_\xi(t)$ as entropy is produced during the irreversible decay of the particle. Note the analogy between excited states and «dissipative structures» introduced in thermodynamics. The excited particle is a nonequilibrium state due to the environment (here the wave packet) and decays when the constraint is released.

4. PRECOLLISIONAL CORRELATIONS AS A FUNCTION OF SPATIAL CONFIGURATION

As follows from the previous discussion, the initial correlations between the particle and the field determine the degree of the order in the system. It is natural to expect that the initial correlations must be larger for higher initial distance between the particle and the wave packet because for the larger distance «targeting» becomes more difficult problem.

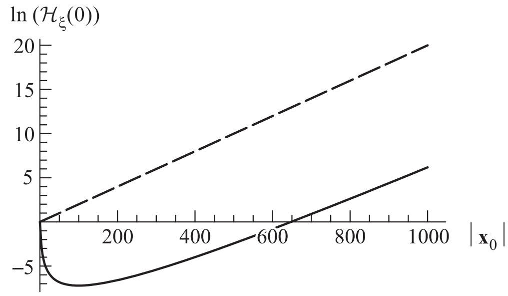

Fig. 3. $\ln(\mathcal{H}_\xi(0))$ as function of $|\mathbf{x}_0|$ for Gaussian wave packets centered in x_0. The size of the wave packet is $a = 1$, and the initial momentum is $k_0 = 1$. Dashed line — 1D; solid line — 3D. The position of the pole is $z_1 = 1 - 0.01i$

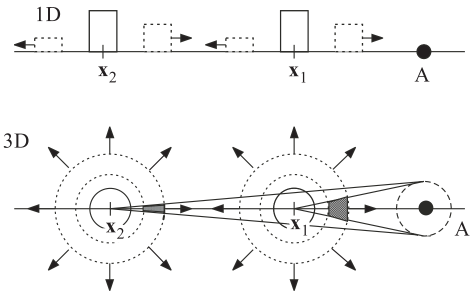

Fig. 4. The origin of initial fall of $\mathcal{H}_\xi$ function with $|\mathbf{x}_0|$: the further is the wave packet, the less portion of it will hit the atom

In order to analyze this, we use the Gaussian wave packet of the size a centered at $\mathbf{x}_0$ with the initial momentum $\mathbf{k}_0$:

$$\langle \mathbf{x}|\xi\rangle = \frac{1}{W^{1/2}} e^{i\mathbf{k}_0\mathbf{x}} \exp\left(-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{2a^2}\right),$$
$$\langle \mathbf{k}|\xi\rangle = \left(\frac{2\omega_{\mathbf{k}}}{W}\right)^{1/2} e^{i(\mathbf{k}-\mathbf{k}_0)\mathbf{x}_0} \exp\left(-\frac{a^2}{2}(\mathbf{k}-\mathbf{k}_0)^2\right). \tag{20}$$

Here, we use bold notations $\mathbf{x}$ and $\mathbf{k}$ in order to distinguish 1D and 3D vectors from their absolute values x and k. For 1D and 3D situations, we have in the continuous limit in the pole approximation

$$\mathcal{H}_\xi(0)|_{1\mathrm{D}} \propto e^{2\gamma|\mathbf{x}_0|}, \quad \mathcal{H}_\xi(0)|_{3\mathrm{D}} \propto \frac{e^{2\gamma|\mathbf{x}_0|}}{(a^4k_0^2 + x_0^2)}. \tag{21}$$

The same result for 1D case was also obtained in [9].

In Fig. 3, we draw $\ln(\mathcal{H}_\xi(0))$ as function of x_0 for 1D (dashed line) and 3D (solid line). The normalization constants are chosen such that for $|\mathbf{x}_0| = 0$ both curves coincide. In both cases, for large $|\mathbf{x}_0|$, due to the factor $e^{2\gamma|\mathbf{x}_0|}$, the entropy exponentially decreases with the distance between the initial position of the wave packet and the atom. The larger the distance $|\mathbf{x}_0|$, the more order (a lower entropy) we must introduce into the system in order to target the wave packet to the particle. However, in 3D, in addition to this effect, we see an initial decrease of $\mathcal{H}_\xi$ function due to the factor $(a^4k_0^2 + x_0^2)^{-1}$ which is absent in 1D.

The origin of this can be explained by simple geometrical reasons (see Fig. 4). In the 3D case, initially localized wave packet spreads in all directions. However the major contribution to $\mathcal{H}_\xi$ is given by those components of the wave packet that have the momenta with the directions in some critical solid angle directed to the atom. This angle becomes nar-

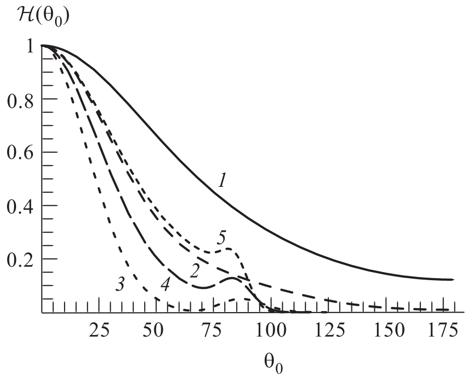

Fig. 5. $\mathcal{H}(\theta_0) \equiv \mathcal{H}_\xi(0)/(\mathcal{H}_\xi(0)|_{\theta_0=0})$ as a function of θ_0 for $x_0 = 10$, $k_0 = \tilde{\omega}_1 = 1$, $\gamma = 0.01$ in the pole approximation. *1* — $a = 1$; *2* — $a = 1.5$; *3* — $a = 4$; *4* — $a = 6$; *5* — $a = 8$

rower with the distance and $\mathcal{H}_\xi$ decreases with $|\mathbf{x}_0|$. This effect dominates at small $|\mathbf{x}_0|$ but for large distances the exponential factor $e^{-2\gamma|\mathbf{x}_0|}$ that is due to interaction starts to overcome the geometrical effect and the $\mathcal{H}_\xi(0)$ curve starts to increase with $|\mathbf{x}_0|$.

Another important question is how pre-collisional correlations depend on whether the wave packet itself is targeted to the atom or not. In Fig. 5, we draw the dependence of $\mathcal{H}_\xi(0)$ on the angle θ_0 between the vector $\mathbf{k}_0$ and the direction from the centre of the wave packet to the atom for different sizes of the wave packet. We see that the $\mathcal{H}_\xi$ function is greater when the wave packet is directed to the atom and becomes smaller with the deviation of $\mathbf{k}_0$ from the direction to the atom. This is in agreement with our statement that when the wave packet is targeted to the atom the order increases.

CONCLUSION

We may summarize the main interest in our $\mathcal{H}$ function as follows:

1) Irreversibility and entropy are not limited to macroscopic physics (contrary to the opinion of Boltzmann). Elementary processes like the decay of an excited state contribute to the entropy balance.

2) The symmetry between incoming waves and outgoing waves as used in S matrix theory is broken (contrary to the opinion of Pauli). Incoming waves have lower entropy.

3) Relation between dynamics (here time inversion) and entropy. On the one hand, velocity inversion leads to the change of entropy. On the other hand, it requires acceleration. Therefore, it is interesting to investigate the relation between acceleration and entropy.

4) Dual aspect of reversible and irreversible processes (according to J. von Neumann) is unified in our formalism in terms of Λ transformation, as it combines both.

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