Quasithermodynamic Representation of the Pauli Markov equation and their possible applications

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We demonstrate that the extensive class of open Markov quantum systems describing by the Pauli master equation can be represented in so-called quasithermodynamic form. Such representation has certain advantages in many respects for example it allows one to specify precisely the parameter region in which the relaxation of the system in question to its stationary state occurs monotonically. With a view to illustrate possible applications of such representation we consider concrete Markov model that has in our opinion self-dependent interest namely the explanation of important and well established by numerous experiments the Yerkes-Dodson law in psychology.

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I. INTRODUCTION

The dynamic equations method is the fundamental tool for studying of the behavior of complex systems in physics, chemistry, population biology and other sciences. This method can be applied both for the deterministic and statistical description for the system in question (in the second case the dynamic equations may be written for the evolution of the probabilities to find the system in all possible states of its phase space). In the paper [1] we had considered one extensive class of dynamical systems so-called quasithermodynamic systems. We define quasithermodynamic system (QS) as the system whose behavior can be characterized by two key functions of its state. By analogy with classical thermodynamics we call these two functions as the energy and entropy. According to definition these two functions must satisfy two main conditions (in the first time introduced in thermodynamics by R. Clausius in 1865, see for example [2]) that look as follows:

I) the energy of QS is constant
II) the entropy of QS monotonically increases in time.

Note that for dynamic equations describing various physical and also nonphysical QS systems the words “energy” and “entropy” should be understand only in the Pickwick sense as conventional labels for two given functions satisfying to above mentioned conditions. In the paper [1] we specify the explicit form of dynamical equations for QS whose states are described by a set of $N$ continuous variables: $x_1, x_2, \ldots, x_N$, and examined some important features of their behavior. The main goal of the present paper to demonstrate that well known Pauli master equation (PME) for diagonal elements of density matrix of some open quantum Markov system can be successfully represented in similar quasithermodynamic form. Such representation brings certain advantages in many respects. In particular as we prove later in this paper it allows one to specify precisely the situations when the QS under consideration tends to its stationary (or equilibrium) state monotonically in time. In addition we consider also one instructive illustration of such representation relating to psychology that in our opinion has self-dependent interest.

The paper is organized as follows. In Sect.1 we briefly remind the necessary facts relating to the theory of QS in particular specify the explicit form of dynamical equations that provide the realization of the Clausius conditions I), II). In Sect.2 that is the central part of the paper we consider the general PME describing the evolution of diagonal elements of expensive class of open quantum Markov systems and demonstrate that it can be represented in required quasithermodynamic form. Note that in the present paper we consider the diagonal elements of density matrix that is the probabilities $p_i$ of finding the system in the state $|i\rangle$ as basic set of variables. In addition the sum of these diagonal elements $\sum_{i=1}^{N} p_i$ will play the role of energy in our case. Evidently that in virtue of normalization condition this sum is conserved and moreover identically equal to unit. The only but nontrivial problem which remains is the problem of the explicit construction of corresponding function of entropy that provides the desired equations of motions for probabilities $p_i$ that is initial PME. Also in this section we specify the conditions which must be imposed on the Markov system of interest in order to provide monotonic damping to its stationary state. In the Sect.3 as some instructive example we study concrete 3 state Markov model that in our opinion explains one important phenomenon in psychology of learning namely the Yerkes-Dodson law. Now let us go to the presentation of concrete results of the paper.

II. PRELIMINARY INFORMATION CONCERNING THE THEORY OF QS

In this part we give the brief account relating to the theory of QS, that is the systems which satisfy the above
two Clausius conditions I),II). The simplest example of QS is the dynamic system whose state is described by two continuous variables \((x_1, x_2)\) and corresponding equations of the motion may be written in the next form:

\[
\frac{dx_i}{dt} = \varepsilon_{ik} \frac{\partial H}{\partial x_k} \{S, H\},
\]

(1)

where \(H(x_1, x_2)\) and \(S(x_1, x_2)\) are two preassigned functions of state, \(\varepsilon_{ik}\) is completely antisymmetric tensor of the second rank and \(\{f, g\} = \varepsilon_{ik} \frac{\partial f}{\partial x_k} \frac{\partial g}{\partial x_k}\) is ordinary Poisson bracket for two functions \(f(x_1, x_2)\) and \(g(x_1, x_2)\). It is easy to see directly that equations of motion Eq. (1) imply the relations: 1) \(\frac{dH}{dt} = 0\) and 2) \(\frac{dS}{dt} = \{S, H\}^2 \geq 0\). Hence the functions \(H\) and \(S\) satisfy to conditions I) - II) and can be considered as "energy" and "entropy" of corresponding QS. Similarly one can write the equations of motions for QS with three variables \(x_1, x_2, x_3\) in the following form:

\[
\frac{dx_i}{dt} = \varepsilon_{ikl} \frac{\partial H}{\partial x_k} A_l,
\]

(2)

where the vector \(A_l = \varepsilon_{lmn} \frac{\partial S}{\partial x_m} \frac{\partial H}{\partial x_n}\) and \(\varepsilon_{ikl}\) is completely antisymmetric tensor of the third rank. Expression Eq. (2) may be rewritten also in the equivalent form:

\[
\frac{dx_i}{dt} = \frac{\partial S}{\partial x_i} \sum_k \left( \frac{\partial H}{\partial x_k} \right)^2 - \frac{\partial H}{\partial x_i} \sum_k \left( \frac{\partial H}{\partial x_k} \frac{\partial S}{\partial x_k} \right).
\]

(3)

However it should be noted that expressions Eq. (2) and Eq. (3) are not the most general form of equations for QS with three variables. In fact we may add in r.h.s of the Eq. (2) the "hamiltonian" term \(-r \varepsilon_{ikl} \frac{\partial S}{\partial x_l} \frac{\partial H}{\partial x_k}\) (where \(r\) is a multiplier) without any changing of its quasithermodynamic character. So the general form of QS with three variables reads as

\[
\frac{dx_i}{dt} = \varepsilon_{ikl} \frac{\partial H}{\partial x_k} \left( A_l - r \varepsilon_{ik} \frac{\partial S}{\partial x_i} \right),
\]

(4)

where the vector \(A_l\) in Eq. (4) is defined in just the same way as in Eq. (2).

The task of description the explicit form of equations of motion for QS with more than three variables in principle can be solved by the same way and we will turn to it a little later. Now let us draw our attention to the other important object of present study namely Pauli master equation (PME). The PME describes the evolution in time the diagonal elements \(P_n\) of density matrix of open quantum Markov system (that is the probabilities to find it in any quantum state \(|n\rangle\)). This equation has the next general form:

\[
\frac{dP_n}{dt} = \sum_m \left( W_{nm} P_m - P_n W_{mn} \right),
\]

(5)

where, \(W_{nm}\) is a probability (per unit time) of transition from quantum state \(|m\rangle\) to state \(|n\rangle\). It is known that Eq. (5) describes both the relaxation of closed Markov system to its equilibrium state and the decay of open system to it nonequilibrium stationary state. In the prominent paper [4] J.S. Tomsen proved some important connections existing between symmetry properties of the coefficients \(W_{nm}\) and the character of corresponding relaxation process described by master equation Eq. (5). For example if coefficients \(W_{nm}\) are symmetric \(W_{nm} = W_{mn}\) then all probabilities \(p^0_{nm}\) in their final stationary state are equal to each other i.e. the ergodic hypothesis in this case holds. Obviously the symmetry condition implies the validity of the detailed balance principle: \(p^0_{nm} W_{mn} = p^0_{mn} W_{nm}\) as well. In addition note that the more weak property of matrix \(W_{nm}\) namely its double stochasticity: \(\sum_{m} W_{nm} = \sum_{m} W_{mn}\) for all indexes \(m\) implies that the Boltzmann-Shennon entropy function \(S_{BS} = -\sum_{i} p_i \ln p_i\) increases in time (that is \(\frac{dS}{dt} \geq 0\)). Thus we can conclude that in symmetric case the PME in fact describes the evolution of the closed quantum system to its equilibrium state.However in our paper we are interested in more general case of open nonequilibrium Markov system when Eq. (5) describes its damping to stationary state as well.So we do not impose in advance any special restrictions on matrix \(W_{mn}\). Now let us turn to our main goal namely to the statement that arbitrary PME can be represented in the form of appropriate QS.

III. THE REPRESENTATION OF THE PME IN QUASITHERMODYNAMIC FORM.

We begin our study with the simplest case of two level open quantum system that can be described by the PME. Then the PME for the diagonal elements of its density matrix \(\hat{\rho}\) namely \(p_1 = \rho_{11}\) and \(p_2 = \rho_{22}\) looks as:

\[
\frac{dp_1}{dt} = W_{12} p_2 - p_1 W_{21},
\]

and

\[
\frac{dp_2}{dt} = W_{21} p_1 - p_2 W_{12}.
\]

(6)

One can easily verify that the system Eq. (6) may be represented in required quasithermodynamic form: \(\frac{d\hat{\rho}}{dt} = \varepsilon_{ik} \frac{\partial H}{\partial x_k} \{\hat{S}, \hat{H}\}\) if we define "energy" \(\hat{H}\) as \(H = p_1 + p_2\) and "entropy" \(\hat{S}\) as \(S = -\frac{W_{12} p_2^2}{1 + p_2} - \frac{W_{21} p_1^2}{1 + p_1}\).

Note if the symmetry condition \(W_{12} = W_{21}\) holds than this "entropy" function in fact coincides with linear Boltzmann-Shennon entropy that provides the relaxation of the system to its equilibrium state with \(p_1^0 = p_2^0 = \frac{1}{2}\). However in general two state Markov system we have for the final probabilities: \(p_1^0 = \frac{W_{12}}{W_{12} + W_{21}}\), and \(p_2^0 = \frac{W_{21}}{W_{12} + W_{21}}\) and ergodic hypothesis does not holds. It is clear that two state case is too simple to shed light on general case but in the next in complexity three-state case all key elements of general construction can be guessed. Therefore we consider this case more detail. For three -level open quantum
system the general PME Eq. (5) can be written in the form
\[
\begin{align*}
\frac{dp_1}{dt} &= -(a + b) p_1 + c p_2 + c p_3 \\
\frac{dp_2}{dt} &= a p_1 - (c + d) p_2 + f p_3 \\
\frac{dp_3}{dt} &= b p_1 + d p_2 - (e + f) p_3
\end{align*}
\] (7)

The full coincidence between the PME Eq. (5) and the system of equations Eq. (7) can be achieved if one introduces the notation: \(a = W_{21}, \ b = W_{31}, \ c = W_{12}, \ d = W_{32}, \ e = W_{13}, \text{ and } f = W_{23}.\)

Note by the way that the general PME for the system with \(N\) basic states obviously has \(N(N - 1)\) independent coefficients so in three state case there are precisely six such parameters.

Now let us seek a representation of the PME in required quasithermodynamic form as
\[
\frac{dp_i}{dt} = \varepsilon_{ikl} \frac{\partial H}{\partial p_k} \left( A_i - r \frac{\partial S}{\partial p_i} \right), \quad (8)
\]
where all indexes take values 1, 2, 3, the vector \(A_i = \varepsilon_{lmn} \frac{\partial S}{\partial p_m} \frac{\partial H}{\partial p_n}, \ H = \sum_{i=1}^{3} p_i \) and \(r\) is some unknown multiplier. Entropy function \(S(p_1, p_2, p_3)\) may be represented as symmetric quadratic form of basic variables \(p_i\) that is
\[
S = \frac{A p_1^2}{2} + \frac{B p_2^2}{2} + \frac{C p_3^2}{2} + \alpha p_1 p_2 + \beta p_1 p_3 + \gamma p_2 p_3 \quad (9)
\]
Note that the transformation: \(S \rightarrow S + k(p_1 + p_2 + p_3)^2\) does not change equations of motion Eq. (8) so without loss of generality we can put the value of \(\gamma\) is equal to zero. Thus in the case of three state Markov system we have six unknown coefficients: \(A, B, C, \alpha, \beta\) and \(r\) that accurately corresponds to six parameters \(a, b, c, d, e, f\) of original PME. Now let us determine the explicit connection between PME Eq. (7) and its representation in quasithermodynamic form Eq. (8). Taking into account the above expression for the vector \(A_i\) one can rewrite Eq. (5) in the next expanded form
\[
\begin{align*}
\frac{dp_1}{dt} &= 2 \frac{\partial S}{\partial p_1} - (1 - r) \frac{\partial S}{\partial p_2} - (1 + r) \frac{\partial S}{\partial p_3} \\
\frac{dp_2}{dt} &= 2 \frac{\partial S}{\partial p_2} - (1 - r) \frac{\partial S}{\partial p_3} - (1 + r) \frac{\partial S}{\partial p_1} \\
\frac{dp_3}{dt} &= 2 \frac{\partial S}{\partial p_3} - (1 - r) \frac{\partial S}{\partial p_1} - (1 + r) \frac{\partial S}{\partial p_2}
\end{align*}
\] (10)

Now substituting the expression Eq. (9) for entropy function \(S\) in r.h.s. of Eq. (10) and compare the result with the PME Eq. (7) after a simple algebra we obtain the next relations for unknown coefficients \(a, b, c,\)
\[
\begin{align*}
\alpha &= \frac{(1 + r) c - (1 - r) d}{3 + r^2}, \\
\beta &= \frac{(1 - r) c - (1 + r) d}{3 + r^2}, \\
B &= \frac{-2d - (1 - r) c}{3 + r^2}, \quad C = \frac{-2f - (1 + r) e}{3 + r^2}.
\end{align*}
\] (11)

Besides we have two additional equations that connect coefficients \(a\) and \(b\) from the PME (7) with unknown coefficients \(A\) and \(r\):
\[
\begin{align*}
a &= 2\alpha - \beta (1 - r) - (1 + r) A \quad (12) \\
b &= 2\beta - \alpha (1 + r) - (1 - r) A.
\end{align*}
\]

Substituting expressions Eq. (11) into Eq. (12) and equating two values for coefficient \(A\) we obtain the final value for the coefficient \(r\). If one introduce the notation \(\kappa = \frac{b + c + f}{a + d + e}\), then the expression for \(r\) reads as \(r = \frac{\sqrt{\kappa} - 1}{\kappa + 1}\). It is obvious that if the condition
\[
a + d + e = b + c + f \quad (13)
\]
is valid (that is \(\kappa = 1\)), the purely "hamiltonian term" \(-r \partial S/\partial p_i \partial p_i\) in quasithermodynamic representation Eq. (8) vanishes. Let us prove now that condition Eq. (13) implies that relaxation of the three state open Markov system to its stationary state occurs monotonically. Indeed if we will seek the solutions of linear PME Eq. (4) in standard form as \(p_i(t) = C_i e^{\lambda t}\) then after the simple algebra we obtain the cubic secular equation for three roots of this equation. One root is precisely equal to zero (since the sum \(\sum_{i=1}^{3} p_i\) is conserved). The other two roots can be obtained from the following quadratic equation:
\[
\lambda^2 + \xi \lambda + (\eta(a + b + e) - (e - c)(f - a)) = 0 \quad (14)
\]
where, \(\xi = a + b + c + d + e + f, \ \eta = c + d + f\). Provided that the determinant of this equation is lesser than zero two roots of Eq. (14) will be real and negative. Thus the necessary and sufficient condition of monotonic relaxation of open Markov system Eq. (7) to its stationary state may be written as
\[
\xi^2 + 4(e - c)(f - a) - 4\eta(a + b + e) \leq 0 \quad (15)
\]
Let us introduce the notation: \(k = e - c, l = f - a, m = b - d\) and \(\omega = (a + d + e) - (b + c + f)\). Then in new notation the condition Eq. (15) looks as \(\omega^2 + 4\omega(l + m) + 4(l^2 + m^2 + lm) \leq 0\) or in more convinient form as
\[
\left(\sqrt{3u + \frac{2}{\sqrt{3}}}\omega\right)^2 + v^2 - \omega^2 \leq 0 \quad (16)
\]
where \(u \equiv l + m\) and \(v \equiv l - m\). We see that the boundary of the region in parameter space of the PME Eq. (7) where the nonmonotonic relaxation of its solution is possible may be represented by the ellipse:
\[
\left(\sqrt{3u + \frac{2}{\sqrt{3}}}\omega\right)^2 + v^2 = \omega^2. \quad \text{Obviously if } \omega = 0, \text{ that is condition } a + d + e = b + c + f \text{ holds, the ellipse degenerates into single point and all solutions of Eq. (7) monotonically decres in time. On the other hand if } \omega \neq 0 \text{ there is a finite region of parameters (the greater the more } \omega \text{ is) where nonmonotonic behavior of solutions of Eq. (7) is possible. So the required result is proved. Now let us}
discuss in short the case of general Markov open system that can be described by PME Eq. (7).

First of all note that above mentioned construction for three state Markov system can be realized with necessary changes in general case as well. We propose here only a short outline of complete proof. So let us consider the N state Markov system that is described by corresponding PME with N(N−1) independent coefficients. We present the QR of the PME for this system in the next schematic form:

\[
\frac{dp_{i_1}}{dt} = \varepsilon_{i_1,i_2} A_{i_1,i_2} + \sum_{\alpha=1}^{(N-1)(N-2)} r_\alpha H_{i_1}^{(\alpha)} \tag{17}
\]

where \(H = \sum_{i=1}^{N} p_i A_{i,i-N} = \varepsilon_{i_1,i_2} A_{i_1,i_2} \frac{\partial S}{\partial p_{i_1}} \frac{\partial H}{\partial p_{i_2}}, \)

\(S(p_1,..p_N)\) is symmetric quadratic form of N variables and \(\varepsilon_{i_1,..i_N}\) is completely antisymmetric tensor of N rank. In addition each of the \((N-1)(N-2)/2\) quasihamiltonian terms \(H_{i_1}^{(\alpha)}\) has the following form:

\[
H_{i_1}^{(\alpha)} = \varepsilon_{i_1,i_2,i_3} A_{i_1,i_2,i_3} \frac{\partial S}{\partial p_{i_2}} \frac{\partial H}{\partial p_{i_3}} \tag{18}
\]

where every antisymmetric tensor \(R_{i_1,i_2,i_3}^{(\alpha)}\) has N−3 rank. The quasihamiltonian representation of Eq. (18) may be constructed by the next procedure. First of all note that above mentioned construction takes into account two successive stage of learning namely a) the primary learning i.e. the transition \([1] = \Rightarrow [2], a\) and b) the secondary or high learning i.e. the transition \([2] \Rightarrow [3], a\) and in addition two destructive transitions that impeding to successful learning c) partial loss of the habit in view of excessive agitation or various external noise i.e. the transition \([3] \Rightarrow [2], a\) and the inevitable forgetting of the habit in view of (for example) long absence from practice i.e. the transition \([3] = \Rightarrow [1], a\).

Now let us formulate the Markov model based on PME that takes into account all above listed reasons. We believe that relevant equations of this model can be written in the following way

\[
\frac{d\rho_1}{dt} = -a\rho_1 + e\rho_3,
\]

\[
\frac{d\rho_2}{dt} = a\rho_1 - d\rho_2 + f\rho_3 \tag{19}
\]

\[
\frac{d\rho_3}{dt} = d\rho_2 - (e+f)\rho_3
\]

where the coefficients a, d, e, f describe the probabilities (per unit time) of above mentioned transitions. We consider \(\rho_i (i=1,2,3)\) as the probabilities to find the individual in corresponding state of learning. Comparing the Eq. (1) with general three state PME Eq. (7) we see that the model proposed Eq. (19) corresponds to its partial case when coefficients \(b = c = 0\). It is easy to see
that the stationary solution of Eq. (19) has the form:

\[
\begin{align*}
\rho_0^1 &= \frac{de}{de + a(d + e + f)}, \\
\rho_0^2 &= \frac{a(e + f)}{de + a(d + e + f)}, \\
\rho_0^3 &= \frac{ad}{de + a(d + e + f)}
\end{align*}
\] (20)

Up to this point we did not take into account the influence of arousal (or motivation) on learning process. Now let us do it. On the grounds of simple psychological reasons we believe that increase of arousal promotes only the transitions \(|1\rangle \Rightarrow |2\rangle\) and \(|3\rangle \Rightarrow |2\rangle\) and has minor effect on transitions \(|3\rangle \Rightarrow |1\rangle\) and \(|2\rangle \Rightarrow |3\rangle\). If we denote the arousal level of training individual (which can be measured by relevant psychological methods as \(k\)), then our assumptions can be explicitely expressed in the form of next two relations: \(a = a_1 k\) and \(f = f_1 k\). Now we believe that coefficients \(a_1, f_1, d, e\) do not depend on arousal. Finally the probability to find the individual in stationary well-trained state can be obtained from Eq. (20) and looks as

\[
\rho^3_0 = \frac{a_1 d k}{de + a_1(d + e)k + a_1 f_1 k^2}
\] (21)

The maximum of expression Eq. (19) is reached when the arousal level is equal to

\[
k_{ext}^2 = \frac{de}{a_1 f_1}.
\] (22)

It is also worth noting that in the cases when the errors in learning can result in grave consequences (for example in such professions as surgeon or pilot) it is highly desirable that the learning process would be consistent. To this end the instructor during the learning process must try to provide the fulfilment of two conditions 1) providing optimal level of motivation that is \(k_{opt} = \sqrt{\frac{de}{a_1 f_1}}\) and 2) that warrants serious failures in training: \(\frac{df}{de} = \frac{f_1 - a_1 f_1}{\sqrt{a_1 f_1}}\). The second of these conditions in fact entirely coincides with condition Eq. (13).

In conclusion of this part we want to emphasize that all results obtained in this simplified model of learning process undoubtely need in careful experimental checking and verification.

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