Generalized Quantum Dynamics with Arrow of Time

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Abstract

It is shown, that quantum theory with complex evolutionary time parameter and non-Hermitian Hamiltonian structure can be used for natural unification of quantum and thermodynamic principles. The theory is postulated as analytical in respect to the parameter of evolution, which real part is identified with the ‘usual’ physical time, whereas the imaginary one is understood as proportional to the inverse absolute temperature. Also, the Hermitian part of the Hamiltonian is put equal to conventional operator of energy. It is shown, that the anti-Hermitian Hamiltonian part, which is taken as commuting with the energy operator, is constructed from parameters of decay of the system. It is established, that quantum dynamics, predicted by this theory, is integrable in the same sense as the corresponding non-modified one, and that it possesses a well defined arrow of time in isothermal and adiabatic regimes of the evolution. It is proved, that average value of the decay operator decreases monotonously (as the function of the physical time) in these important thermodynamical regimes for the arbitrary initial data taken. We discuss possible application of the general formalism developed to construction of time-irreversible modification of a string theory.

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1 Introduction

Irreversibility of evolution is a common feature of all real dynamical systems. This fact is reflected in the second law of thermodynamics, which states that entropy of any closed physical system can not decrease. Figuratively, one says about ‘arrow of time’, which separates past and future in absolute manner, and must be guaranteed by any realistic dynamical theory without fail [1]–[4].

It is important to stress, that thermodynamics itself is not a dynamical theory of the same type as, for example, classical or quantum mechanics. Rather, it provides general theoretical framework for dynamical theories, which pretend to adequate description of evolving physical reality. Also, it can be said, that thermodynamical principles must be realized on the base of consistent dynamical theory of fundamental type, and that the thermodynamics imposes hard restrictions to the corresponding theoretical constructions [5].

In this connection, one must take into account, that all quantum and classical fundamental theories are conservative Hamiltonian systems [6]–[7]. All these systems are reversible in time, because one can interchange their initial and final data to obtain really possible result of the dynamical evolution. Thus, these theories, being the most natural concrete classes of the closed dynamical systems, can not be used for any consistent realization of thermodynamic conception of the arrow of time. All attempts performed to ‘average out’ the reversible results of these theories to obtain the thermodynamic irreversible ones, contain hidden incorrect actions. For example, impossibility to consider unidirectional evolution in framework of classical mechanics can be understood using results of the Poincare theorem. Actually, it states, that one can decompose any classical motion to the set of ‘Poincare cycles’, so this motion obtains transparently reversible character. The same situation takes place in the quantum mechanics: using the Hamiltonian proper basis, one reduces the quantum motion to the set of corresponding oscillations, which are reversible in time manifestly. Also, probabilities to find quantum system in the Hamiltonian eigenstates remain constant quantities, and one can not relate any irreversible dynamics of the kinetic type to them.

It is important to emphasize, that the set of conventional kinetic equations contain arrow of time by its definition. Such equations had been used extensively by Prigogine in his study of both thermodynamic and synergetic processes [8]. The only conceptual problem of such approaches is how to ground the kinetic method of realization of the time irreversible disciplines on the fundamental level in the really correct form. In the over words, one must show how to modify the fundamental theories of the classical and quantum mechanical types to achieve their consistency with the conventional kinetic framework. In this paper we answer on this question by presentation of some ‘minimal’ generalization of the quantum theory. The corresponding modification of the classical theory will be developed in forthcoming
publications.

Our generalization of the conservative quantum theory is related to use of complex parameter of the evolution (or ‘complex time’, see [9]–[12]), and non-Hermitian Hamiltonian operator independent on this parameter [13]–[16]. Also, we suppose analytic dependence of quantum states of the theory on the complex time, and impose commutativity restriction on the Hamiltonian and result of its Hermitian conjugation. We interpret the real part of the complex time as ‘usual’ physical time, whereas the imaginary one we identify as proportional to the inverse absolute temperature of the system. Then, the Hermitian part of the Hamiltonian we put equal to energy operator of this quantum system, whereas the anti-Hermitian part is naturally related to operator of decay parameters of the energy eigenstates. Finally, we define thermodynamic regimes of the evolution: this allows us to determine temperature functions for concrete thermodynamic processes considered. It is shown, that quantum dynamics, predicted by the theory, has a well defined arrow of time in the isothermal and adiabatic regimes of the evolution.

2 Generalized quantum theory

It seems clear, that any realistic generalization of the quantum theory must start with some complex linear space of state vectors $\Psi_1, \Psi_2, \text{etc.}$, and some well-defined scalar products $\Psi_1^+ \Psi_2, \text{etc.}$, of these vectors. Moreover, one must preserve a probability interpretation of the theory. For example, in the normalizable case, one must use the relation

$$P = \frac{\Psi_1^+ \Psi_2 \cdot \Psi_1^+ \Psi_1}{\Psi_1^+ \Psi_1 \cdot \Psi_2^+ \Psi_2} \quad (2.1)$$

for the probability $P$ to find the system in the condition with the state vector $\Psi_1$, if this system is specified by the state vector $\Psi_2$. Then, it is necessary to deal with some set of the observables $Q_1, Q_2, \text{etc.}$, which are linear Hermitian operators acting on the state vectors. Without any doubt, a rule for calculation of the average value $\bar{Q}$ for the observable $Q$, which is related to the state vector $\Psi$, must save its well-known conventional form:

$$\bar{Q} = \frac{\Psi^+ Q \Psi}{\Psi^+ \Psi}. \quad (2.2)$$

Also, the average values must preserve their meaning in relation of results of the quantum theory to the corresponding observations in the real world.

Then, all dynamical aspects of generalized quantum theory must be described in terms of some evolutionary parameter $\tau$ and Hamiltonian operator $\mathcal{H}$. For natural analogies of
conservative systems, one must put $\mathcal{H}_\tau = 0$ in the Schrödinger’s picture (which we explore in this work). Also, the main dynamical equation of the theory must preserve its conventional Schrödinger’s form,

$$i\hbar \Psi, \tau = \mathcal{H}\Psi.$$  \hspace{1cm} (2.3)

Note, that all elements of the quantum theory listed above are completely standard ones.

Our modification of this theory is based on the use of the complex time parameter $\tau \neq \tau^*$ and non-Hermitian Hamiltonian operator $\mathcal{H} \neq \mathcal{H}^+$. We consider a holomorphic variant of the theory, with $\Psi, \tau^* = 0$ and $\mathcal{H}, \tau^* = 0$, which leads to the simplest generalization of the standard theoretical quantum scheme. We restrict our consideration by the theories with $[\mathcal{H}, \mathcal{H}^+] = 0$. The last relation becomes an identity in the standard theory case, when $\mathcal{H} = \mathcal{H}^+$, so one can really speak about the ‘minimal generalization’. We parameterize the complex evolutionary parameter $\tau$ in terms of the real variables $t$ and $\beta$ in the following form:

$$\tau = t - i\frac{\hbar}{2\beta},$$  \hspace{1cm} (2.4)

whereas the non-Hermitian operator $\mathcal{H}$ will be represented using the Hermitian ones $E$ and $\Gamma$ as

$$\mathcal{H} = E - i\frac{\hbar}{2\Gamma}.$$  \hspace{1cm} (2.5)

Note, that

$$[E, \Gamma] = 0,$$  \hspace{1cm} (2.6)

in accordance to the restriction imposed above. In the next section we will argue, that, if one identifies the quantities $t$ and $E$ with the ‘usual’ time and energy operator, respectively, then the remaining quantities $\beta$ and $\Gamma$ mean the inverse absolute temperature $\beta = 1/kT$ (multiplied to the Bolzman constant $k$), and the operator of inverse decay time parameters of the system. Also, it will be demonstrated, that the former operator defines an arrow of time, which seems naturally in view of transparent irreversibility of any decay process.

Then, this scheme of generalization of the quantum theory must be completed by introducing of a conception of thermodynamic regime, which has a form of fixation of the temperature function $\beta = \beta(t)$. For example, one can study evolution of the system in the isothermal case $\beta = \text{const}$. Also, it is possible to analyze the adiabatic situation with $\dot{E}(t, \beta) = \text{const}$ (the system under consideration does not perform a work, because $\mathcal{H}$ is
time-independent, so this regime is adiabatic actually). The most general thermodynamic regime, which is related to the observable $Q$, can be defined as

$$f \left( t, \beta, \bar{Q}(t, \beta) \right) = 0.$$  \hspace{1cm} (2.7)

In this work we would like to show, that the modified quantum theory presented above possesses a well defined arrow of time in the isothermal and adiabatic regimes of its thermodynamical evolution.

3 Time, energy, temperature and parameters of decay

So, our main goal is to detect and to study irreversible aspects of evolution of the generalized quantum system, defined in the previous section. To do it in explicit form, let us express all significant quantities of the theory in terms of a common basis of the eigenvectors $\psi_n$ of the commuting operators $E$ and $\Gamma$. We take it in orthonormal form (i.e., we mean that the identities $\psi_n^+ \psi_k = \delta_{nk}$ take place). Here, of course, the indexes are understood in the appropriate multi-index sense (and all summations have the corresponding type). The eigenvalue problem under consideration reads:

$$E\psi_n = E_n \psi_n, \quad \Gamma\psi_n = \Gamma_n \psi_n; \hspace{1cm} (3.1)$$

it can be reformulated in terms of the non-Hermitian operator $\mathcal{H}$. Actually, it is easy to see, that $\psi_n$ is the eigenvector for this operator, which corresponds to the complex eigenvalue $\mathcal{H}_n = E_n - i\hbar/2\Gamma_n$. Then, the state vectors $\Psi_n = e^{-i\mathcal{H}_n\tau/\hbar}\psi_n$ satisfy the Schrödinger’s equation (2.3), and also form the complete (but $\tau$-dependent) basis. This basis can be used for representation of any solution $\Psi$ of the Schrödinger’s equation in the form of linear combination with some set of constant parameters $C_n$, i.e., as

$$\Psi = \sum_n C_n \Psi_n. \hspace{1cm} (3.2)$$

Using this decomposition formula and the orthonormal basis properties, one can calculate the probability $P_n$ to find the quantum system in its basis state $\Psi_n$, when it is described by the state vector $\Psi$. After the application of Eq. (2.1) one obtains, that

$$P_n = \frac{w_n}{Z}, \hspace{1cm} (3.3)$$

where $Z = \sum_n w_n$,

$$w_n = \rho_n e^{-(E_n\beta + \Gamma_n t)}, \hspace{1cm} (3.4)$$
and $\rho_n = |C_n|^2$. Note, that all following analysis will be related to study of dynamics of the probabilities (3.3)–(3.4) in different thermodynamical regimes and for various special realizations of the generalized quantum theory. In this analysis, the formula (3.4) provides the base for both theoretical and experimental study of the our generalization approach comparing with the standard quantum theory.

First of all, let us consider evolution of two very special systems, which dynamical properties can explain our interpretation of the imaginary part of the complex time parameter $\tau$, and the anti-Hermitian part of the Hamiltonian operator $\mathcal{H}$. Namely, our first system has coinciding eigenvalues $\Gamma_n$ for the all indexes $n$ (i.e., this system is ‘decay-free’, in fact). It is easy to see, that

$$w_n = \rho_n e^{-E_n \beta}$$

in this case. This formula demonstrates, that the quantity $\beta$ is actually the inverse absolute temperature (multiplied to the Boltzman constant), if $E_n$ is identified with the $n$-th ‘energy level’ of the system.

The second special system is specified by coinciding eigenvalues $E_n$ of the energy operator (i.e., dynamics of this system is defined by the operator $\Gamma$ only). Then, $w_n = \rho_n e^{-\Gamma_n t}$ in this case, so the quantities $\Gamma_n$ have the sense of decay parameters, if $t$ means the conventional (‘usual’) physical time. Actually, let us consider, for example, the system with

$$\Gamma_{n^*} = \min_n \{\Gamma_n\} = 0$$

in the situation, where the single level $n$ is weakly excited under the level $n^*$ (in fact, these ‘levels’ are the corresponding solution subspaces). In this special case, $\rho_m = \rho_n \delta_{mn}$, where $n, m \neq n^*$, and also $\rho_{n^*} \approx 1$, whereas $\rho_m \approx 0$ (because $\rho_m << \rho_{n^*}$). It is easy to see, that for this weakly excited quantum state,

$$P_m \approx \rho_m e^{-\Gamma_m t},$$

so $t_m = 1/\Gamma_m$ is a conventional ‘time of life’ for the excitation under consideration, if $t$ has the standard time interpretation. Also, it is clear, that the subspace marked by the index $n^*$ plays an attractor role in the dynamics of the second special system. Note, that in the same situation with $\Gamma_{n^*} = \max_n \{\Gamma_n\}$, one deals with the exponentially increasing probability $P_m(t)$. However, we use the term ‘parameter of decay’ for the quantity $\Gamma_n$ in all regimes of the evolution.

Then, the solution space of the theory of a discussing type can be decomposed into the direct sum of the subspaces, which have a given value of the energy or of the parameter of
decay. For all these subspaces, the interpretation of $\beta$ and $\Gamma_n$ is the same one, as for the special systems of the first and second discussed types, respectively. Finally, we extend the interpretation of these physical quantities (as well as the interpretation of the quantities $E$ and $t$) to the total solution space of the generalized quantum theory, making a simple and natural fundamental generalization.

4 Quantum (thermo)dynamics and arrow of time

Now let us consider non-specified quantum theory of the form, presented in the previous sections, and study the isothermal regime of its thermodynamical evolution. It is easy to prove, that in the case of $\beta = \text{const}$, the dynamical equation for the basis probabilities reads:

$$\frac{dP_n}{dt} = -\left(\Gamma_n - \bar{\Gamma}\right) P_n.$$  \hspace{1cm} (4.1)

To perform its analysis, let us study a behavior of the quantity $\bar{\Gamma}$. After some calculations one obtains, that

$$\frac{d\bar{\Gamma}}{dt} = -D_\Gamma^2,$$  \hspace{1cm} (4.2)

where $D_\Gamma^2 = (\Gamma - \bar{\Gamma})^2$ is the squared dispersion of the quantum observable $\Gamma$. From Eq. (4.2) it follows, that the function $\bar{\Gamma}(t)$ is not increasing. This means, that the isothermal regime of evolution has arrow of time. It is seen, that this can be related to the average value of the decay operator of this quantum system.

Then, the probability $P_n$ rises, if $\bar{\Gamma} > \Gamma_n$, and degenerates, when $\bar{\Gamma} < \Gamma_n$. Thus, in the isothermal case, the quantity $|\Gamma_n - \bar{\Gamma}|$ has a sense of the inverse time of exponential growth or degeneration of the probability to find the system in the subspace of eigenstates with the given value $\Gamma_n$ of the decay operator $\Gamma$. Also, in this regime, one obtains the following picture for asymptotics of the probabilities: all ‘activated’ probabilities (with $\rho_n \neq 0$) with the maximal value of the decay parameter rise droningly, whereas all the remaining probabilities fall to the zero values. The non-activated probabilities (with $\rho_n = 0$) remain trivial during all dynamic history of the system.

Actually, let us define the multi-index $n_*$ by the relation (3.6), again. Then, for the only non-degenerating (at $t \to +\infty$) probabilities $P_{n_*}$, one obtains the following asymptotical result:

$$P_{n_*}(+\infty) = \Pi P_{n_*}(0),$$  \hspace{1cm} (4.3)
where the scale parameter $\Pi > 1$ reads:

$$
\Pi = 1 + \frac{\sum_{n \neq n_0} \rho_n e^{-E_n \beta}}{\sum_n \rho_n e^{-E_n \beta}}.
$$

(4.4)

Note, that the relations (4.3)–(4.4) have a form of ‘dressing procedure’ in standard quantum field theory. This circumstance seems really hopeful in context of solution of different problems related to its renormalization. Roughly speaking, in such theories one deals with infinite set of oscillating harmonics (in the corresponding representation on shell). Then, one needs in cut of this infinity to reach a theoretical scheme with really consistent calculations. However, all known cut procedures are in contradiction with ‘all normal neglecting principles’. The generalized quantum theory presented above allows one to work with the modes, which degenerate dynamically, and also with the ones, which remain ‘alive’ at the ‘big times’. Moreover, these former modes of the exact quantum theory solution become renormalized during the total dynamical history of the system, as it follows from comparison of values for their initial and final probabilities (see Eqs. (4.3)–(4.4)).

Then, it is easy to prove, that in the general case of $\beta = \beta(t)$, the dynamical equations for the basis probabilities have the following form:

$$
\frac{dP_n}{dt} = -\left[\Gamma_n - \Gamma + (E_n - \bar{E}) \frac{d\beta}{dt}\right] P_n.
$$

(4.5)

Here, the specific function $d\beta/dt$ must be extracted from the corresponding thermodynamical regime (2.7). In the adiabatic case, when $\bar{E} = \sum_n E_n P_n = \text{const}$, one obtains immediately, that

$$
\frac{d\beta}{dt} = -\frac{ET - \bar{E}\Gamma}{D^2_E},
$$

(4.6)

where $D_E$ denotes a dispersion of the energy operator $E$. Using Eqs. (4.5)–(4.6), one obtains for dynamics of the quantity $\bar{\Gamma}$ in the adiabatic regime, that

$$
\frac{d\bar{\Gamma}}{dt} = -D^2_{\bar{\Gamma}} \left[1 - \frac{(ET - \bar{E}\Gamma)^2}{D^2_E D^2_{\bar{\Gamma}}}\right].
$$

(4.7)

Our goal is to show, that the function $\bar{\Gamma}(t)$ is non-increasing again, so the system under consideration has a well-defined arrow of time in the adiabatic regime of evolution too. To do it, let us show that the expression [...] in Eq. (4.7) is not negative. Let us introduce the
formal vector quantities $X$ and $Y$ with the components $X_n = E_n - \bar{E}$ and $Y_n = \Gamma_n - \bar{\Gamma}$, and the scalar product $(XY) = \sum_n P_n X_n Y_n$ of these vectors. It is not difficult to prove, that in terms of these quantities, the expression under consideration has the following form: 

$$[...] = 1 - (XY)^2/[(XX)(YY)].$$

Thus, it is actually non-negative – in view of general Cauchy-Buniakowski inequality, which can be applied to its estimation.

## 5 Conclusion

Thus, in the isothermal and adiabatic regimes of the thermodynamical evolution, the generalized quantum dynamics developed in this work has a well-defined arrow of time. Note, that these regimes are the most important ones for the particle physics and cosmological applications of the theory [19]. In the particle physics case, one can take the decay operator in its parity form. Then, one will deal with the system with pure dynamical mechanism of the left-right asymmetry production, which seems much more natural than the standard parity violation scheme. In the cosmological case, the real presence of the arrow of time in the theory seems necessary ‘up to definition’. However, the standard cosmology derived from the General Relativity (or from its supergravity and superstring modifications) is described by time-reversible equations of motion. It is clear, that one needs in fundamental generalization of the theoretical scheme to achieve consistence of cosmology with the second law of thermodynamics. In this paper, we have proposed the ‘minimal quantum theory framework’ for the such modification.

We think, that the approach developed above must be applied for corresponding reformulation of the string theory. In addition to the ‘renormalization arguments’ presented in the section 4 (see Eq. (4.4)), also one has ‘pure thermodynamical reasons’ for the such string theory generalization. Actually, in string gravity models, black hole solutions admit the standard thermodynamical interpretation, related to the Hawking’s correspondence between horizon area and entropy of the black hole. Moreover, in the string theory this correspondence obtains its fundamental statistical ground: one can calculate all necessary macroscopic quantities by counting of their microscopic realizations. Thus, the string theory itself provides necessary ‘kinematical base’ for the conventional thermodynamical evolution. However, string theory equations of motion are time-reversible, so its ‘thermodynamical kinematics’ does not support by ‘thermodynamical dynamics’. We think, that the string theory modification in the direction developed in this paper can improve this non-natural situation. The resulting stringy cosmology and black hole physics will in complete agreement with the standard thermodynamics with the arrow of time.

At the end of this paper we would like to stress, that in the modified quantum theory
under consideration, the symmetry operator $\Gamma$ (it is taken as commuting with the Hamiltonian of the system) does not define any conserved quantity. This interesting property of the quantum theory also must take place in its classical limit (we hope to demonstrate it in the forthcoming publication). Thus, our generalization of the theory in the direction of its irreversibility destroys the well known relation between symmetries and integrals of motion, which is stated by the famous Noether’s theorem.

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