Automatic hermiticity for mixed states

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We previously proposed a mechanism to effectively obtain, after a long time development, a Hamiltonian being Hermitian with regard to a modified inner product \( I_Q \) that makes a given non-normal Hamiltonian normal by using an appropriately chosen Hermitian operator \( Q \). We studied it for pure states. In this letter we show that a similar mechanism also works for mixed states by introducing density matrices to describe them and investigating their properties explicitly both in the future-not-included and future-included theories. In particular, in the latter, where not only a past state at the initial time \( T_A \) but also a future state at the final time \( T_B \) is given, we study a couple of candidates for it, and introduce a “skew density matrix” composed of both ensembles of the future and past states such that the trace of the product of it and an operator \( O \) matches a normalized matrix element of \( O \). We argue that the skew density matrix defined with \( I_Q \) at the present time \( t \) for large \( T_B - t \) and large \( t - T_A \) approximately corresponds to another density matrix composed of only an ensemble of past states and defined with another inner product \( I_{Q_J} \) for large \( t - T_A \).

1. Introduction

Quantum theory is described well via the Feynman path integral. In the Feynman path integral, the action in the integrand is considered to be path-dependent, while the measure is usually supposed to be path-independent. However, we could consider a theory such that not only the action but also the measure is path-dependent. This is the complex action theory (CAT) whose action is complex at a fundamental level but expected to look real effectively [1]. The CAT provides us with falsifiable predictions [1–4]. Deeper understanding via the CAT have been tried even for the Higgs mass [5], quantum mechanical philosophy [6–8], some fine-tuning problems [9,10], black holes [11], de Broglie–Bohm particles and a cut-off in loop diagrams [12], a mechanism to obtain Hermitian Hamiltonians [13], the complex coordinate formalism [14], and the momentum relation [15,16]. There are two types of CAT. One is the future-not-included theory, where only the past state \( |A(T_A)\rangle \) at the initial time \( T_A \) is given and the time integration is performed over the period from \( T_A \) to a reference time \( t \). The other is the future-included one, where not only the past state \( |A(T_A)\rangle \) but also the future state \( |B(T_B)\rangle \) at the final time \( T_B \) is given, and the time integration is performed over the whole period from \( T_A \) to \( T_B \).
We elucidated various interesting properties of the future-not-included CAT \[16\]. In Ref. [17] we argued that, if a theory is described with a complex action, then such a theory is suggested to be the future-included theory, rather than the future-not-included one, as long as we respect objectivity. Even so, the future-not-included CAT itself still remains a fascinating theory, and a good playground to study various intriguing aspects of the CAT.

In the future-included theory, the normalized matrix element \( \langle \hat{O} \rangle^{BA} = \langle B(t) | \hat{O} | A(t) \rangle / \langle B(t) | A(t) \rangle \) of an operator \( \hat{O} \) is expected to have the role of an expectation value [1]. Indeed, if we regard it so, we can obtain nice properties such as the Heisenberg equation, Ehrenfest’s theorem, and a conserved probability current density [21,22]. However, \( \langle \hat{O} \rangle^{BA} \) is generically complex even for Hermitian \( \hat{O} \), even though any observables are real. To resolve this problem, in Refs. [23,24], we proposed a theorem that states that, provided that an operator \( \hat{O} \) is \( Q \)-Hermitian, i.e., Hermitian with regard to a modified inner product \( I_Q \) that makes a given non-normal Hamiltonian \( \hat{H} \) normal by using an appropriately chosen Hermitian operator \( Q \), the normalized matrix element defined with \( I_Q \) becomes real and time-develops under a \( Q \)-Hermitian Hamiltonian for the past and future states selected such that the absolute value of the transition amplitude defined with \( I_Q \) from the past state to the future state is maximized. We call this way of thinking the maximization principle. We proved the theorem in the case of non-normal Hamiltonians \( \hat{H} \) [23] and in the real action theory (RAT) [24]. In addition, we studied the periodic CAT and proposed a variant type of the maximization principle, by which the period could be determined [32].

The maximization principle is based on the natural way of thinking and looks promising. Behind the principle, the automatic hermiticity mechanism [13] has a key role. In the CAT the imaginary parts of the eigenvalues \( \lambda_i \) of a given non-normal Hamiltonian \( \hat{H} \) are supposed to be bounded from above for the Feynman path integral \( \int e^{i\hat{H} S} D\text{path} \) to converge. Then we can imagine that some \( \text{Im} \lambda_i \) take the maximal value \( B \), and denote the corresponding subset of \( \{ i \} \) as \( A \). After a long time development, only the subset \( A \) contributes most significantly, and on the subset a \( Q \)-Hermitian Hamiltonian effectively emerges. This is the automatic hermiticity mechanism that we proposed and studied explicitly for pure states time-developing forward [13]. In Ref. [21], utilizing it for pure states time-developing forward and backward, we showed that the normalized matrix element of \( \mathcal{O} \) at the present time \( t \) in the future-included theory for large \( T_B - t \) and large \( t - T_A \) corresponds to the expectation value of \( \mathcal{O} \) in the future-not-included theory defined with a modified inner product \( I_Q \) for large \( t - T_A \). This study strongly suggests that the future-included CAT is not excluded phenomenologically, even though it looks very exotic. The automatic hermiticity mechanism has an essential role for the CAT to be viable, but so far we have studied it only for pure states, not for mixed states. Thus it would be natural to pose the question: how does it work for mixed states? Even though mixed states can always be expressed by pure states defined in a larger system that includes the mixed states in its subsystem, it is interesting and worthwhile to study how mixed states are defined and how they behave in the CAT. In particular, it is intriguing to study the automatic hermiticity mechanism

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1The normalized matrix element \( \langle \hat{O} \rangle^{BA} \) is called the weak value [18,19] and has been studied intensively with a different philosophy in the real action theory (RAT). For details, see Ref. [20] and references therein.

2The Hamiltonian \( \hat{H} \) is generically non-normal, so it is not restricted to the class of PT-symmetric non-Hermitian Hamiltonians that were studied in Refs. [25–29].

3The proof is based on the existence of imaginary parts of the eigenvalues of \( \hat{H} \), so it cannot be applicable to the RAT case. The maximization principle is reviewed in Refs. [30,31].
for mixed states in the CAT, because the emergence of a Hermitian Hamiltonian is crucially important for the CAT to be sensible, and also because mixed states are generic quantum states along with pure states.

We need to introduce density matrices to describe mixed states in the CAT. In the future-not-included CAT, there is only one class of state vectors time-developing forward from the past, while in the future-included CAT there are two classes of state vectors time-developing not only forward but also backward from the future. Hence it would be more non-trivial to define density matrices and see the emergence of hermiticity for them in the future-included CAT rather than the future-not-included one. Therefore, in this letter, after reviewing the modified inner product $I_Q$ and automatic hermiticity mechanism for pure states, we first define density matrices to describe mixed states and study the emergence of hermiticity for them in the future-not-included CAT. Next, we investigate a couple of candidates for density matrices in the future-included CAT, and introduce a “skew density matrix” composed of both ensembles of the future and past states such that the trace of the product of it and an operator $\mathcal{O}$ becomes a normalized matrix element of $\mathcal{O}$. Furthermore, we argue that the skew density matrix defined with $I_Q$ at the present time $t$ for large $T_B - t$ and large $t - T_A$ approximately corresponds to another type of density matrix composed of only an ensemble of the past state and defined with another inner product $I_Q^\ast$, for large $t - T_A$. Finally we summarize the study in this letter and discuss the outlook of our theory.

2. Modified inner product and the automatic hermiticity mechanism for pure states

In this section we briefly review the modified inner product $I_Q$ and the automatic hermiticity mechanism for pure states by following Refs. [13,14]. The eigenstates of a given non-normal Hamiltonian $\hat{H}$, $|\lambda_i\rangle (i = 1, 2, \ldots)$ obeying $\hat{H}|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$, are not orthogonal to each other in the usual inner product $I$. Let us introduce a modified inner product $I_Q$ [13,14] such that $|\lambda_i\rangle (i = 1, 2, \ldots)$ become orthogonal to each other with regard to it, i.e., for arbitrary kets $|u\rangle$ and $|v\rangle$, $I_Q(|u\rangle, |v\rangle) \equiv (|u\rangle_{Q^\ast}|v\rangle) \equiv (|u\rangle_{Q}|v\rangle)$, where $Q$ is a Hermitian operator that obeys $\langle \lambda_i | Q | \lambda_j \rangle = \delta_{ij}$. Using the diagonalizing operator $P = (|\lambda_1\rangle, |\lambda_2\rangle, \ldots)$ such that $P^{-1} \hat{H} P = D = \text{diag}(\lambda_1, \lambda_2, \ldots)$, we choose $Q = (P^T)^{-1} P^{-1}$. Next we define the $Q$-Hermitian conjugate $Q^\ast$ of an operator $A$ by $\langle \psi_2 | Q^\ast A | \psi_1 \rangle^* = \langle \psi_1 | A Q | \psi_2 \rangle$, so $A^\ast Q^\ast Q^{-1} = Q^{-1} A^\ast Q$. If $A^\ast Q^\ast Q$ is Hermitian, we also introduce $Q^\ast$ for kets and bras as $|\lambda\rangle^\ast = (|\lambda\rangle)_{Q^\ast}$ and $(|\lambda\rangle_{Q^\ast})^\ast = |\lambda\rangle$. Then, since $P^{-1} = P^\ast |Q^\ast\rangle$, $\hat{H}$ is $Q$-normal, $[\hat{H}, \hat{H}^\ast_{Q^\ast}] = 0$. We can decompose $\hat{H}$ as $\hat{H} = \hat{H}_{Qh} + \hat{H}_{Qa}$, where $\hat{H}_{Qh} = \frac{\hat{H} + \hat{H}^\ast_{Q^\ast}}{2}$ and $\hat{H}_{Qa} = \frac{\hat{H} - \hat{H}^\ast_{Q^\ast}}{2}$ are $Q$-Hermitian and anti-$Q$-Hermitian parts of $\hat{H}$, respectively.

Let us consider a state $^5 |A_i(t)\rangle$, which obeys the Schrödinger equation

$$i\hbar \frac{d}{dt} |A_i(t)\rangle = \hat{H} |A_i(t)\rangle. \quad (1)$$

We introduce a normalized state and an expectation value of an operator $\mathcal{O}$ by $|A_i(t)\rangle_N = \frac{1}{\sqrt{|A_i(t)\rangle_Q \langle A_i(t)|}} |A_i(t)\rangle$, $\langle \mathcal{O} \rangle_{A_i(t)}^{A_i(t)} \equiv N \langle A_i(t)|_Q \mathcal{O} |A_i(t)\rangle_N$. They obey $i\hbar \frac{d}{dt} |A_i(t)\rangle_N = \hat{H}_{Qh}|A_i(t)\rangle_N + \hat{A} (\hat{H}_{Qh}; |A_i(t)\rangle_N) |A_i(t)\rangle_N$, $\frac{d}{dt} \langle \mathcal{O} \rangle_{A_i(t)}^{A_i(t)} = -\frac{i}{\hbar} \{ \hat{\mathcal{O}}, \hat{H}_{Qh} \}^{A_i(t)}_{A_i(t)} - \frac{\lambda_i}{\hbar} \{ \hat{\mathcal{O}}, \hat{A} (\hat{H}_{Qh}; |A_i(t)\rangle_N) \}^{A_i(t)}_{A_i(t)}$, where we have introduced $\hat{A} (\hat{H}_{Qh}; |A_i(t)\rangle_N) = \hat{H}_{Qa} - N (|A_i(t)\rangle_{Q^\ast} \langle \hat{H}_{Qa} |A_i(t)\rangle_N)$. It seems that, in the classical limit, since $\left\{ \hat{\mathcal{O}}, \hat{A} (\hat{H}_{Qh}; |A_i(t)\rangle_N) \right\}^{A_i(t)}_{A_i(t)}$
is suppressed, $\langle \hat{O} \rangle_Q^{A_i A_j}(t)$ time-develops by a $Q$-Hermitian Hamiltonian, and Ehrenfest’s theorem holds. This property is intriguing, but we will see the emergence of the $Q$-hermiticity even before considering the classical limit via the automatic hermiticity mechanism, which we explain below.

Expanding $|A_i(t)\rangle$ as $|A_i(t)\rangle = \sum_j a_j^{(i)}(t)|\lambda_j\rangle$ and introducing $|A_i'(t)\rangle = P^{-1}|A_i(t)\rangle = \sum_j a_j^{(i)}(t)|e_j\rangle$, which obeys $i\hbar \frac{d}{dt}|A_i'(t)\rangle = D|A_i'(t)\rangle$, we obtain $|A_i(t)\rangle = Pe^{i\frac{\hat{H}}{\hbar}D(t-t_0)}|A_i'(t_0)\rangle = \sum_j a_j^{(i)}(t_0)e^{i\frac{\pi}{4} (\text{Im} \lambda_j - \text{Re} \lambda_j)\lambda_j\langle\lambda_j|}$. Now we assume that the anti-$Q$-Hermitian part of $\hat{H}$ is bounded from above for the Feynman path integral $\int e^{i\frac{\pi}{4} S\hat{D}}$ path to converge. Based on this assumption we can imagine that some $\text{Im} \lambda_j$ take the maximal value $B$, and denote the corresponding subset of $\{j\}$ as $A$. After a long time has passed, i.e., for large $t - t_0$, the states with $\text{Im} \lambda_j |\in A$ contribute most in the sum. Let us define a diagonalized Hamiltonian $\hat{D}_R$ by

$$\langle e_j|\hat{D}_R|e_k\rangle \equiv \begin{cases} \langle e_j|D_R|e_k\rangle = \delta_{jk} \text{Re} \lambda_j & \text{for } j \in A, \\ 0 & \text{for } j \notin A, \end{cases}$$

and introduce $\hat{H}_{\text{eff}} \equiv P\hat{D}_R P^{-1}$. Since $(\hat{D}_R)^\dagger = \hat{D}_R$, $\hat{H}_{\text{eff}}$ is $Q$-Hermitian, $\hat{H}_{\text{eff}}^\dagger = \hat{H}_{\text{eff}}$, and satisfies $\hat{H}_{\text{eff}}|\lambda_j\rangle = \text{Re} \lambda_j|\lambda_j\rangle$. Then $|A_i(t)\rangle$ is evaluated as $|A_i(t)\rangle \simeq e^{i\frac{\pi}{4} B(t-t_0)} \sum_{j \in A} a_j^{(i)}(t_0)e^{-\frac{\pi}{4} \lambda_j} |\lambda_j\rangle = e^{i\frac{\pi}{4} B(t-t_0)} e^{-\frac{\pi}{4} \hat{H}_{\text{eff}}(t-t_0)}|\Lambda_i(t_0)\rangle = |\Lambda_i(t)\rangle$, where we have introduced $|\Lambda_i(t)\rangle \equiv \sum_{j \in A} a_j^{(i)}(t)|\lambda_j\rangle$. Since the factor $e^{i\frac{\pi}{4} B(t-t_0)}$ is dropped out for the normalized state $|A_i(t)\rangle_N$, we have effectively obtained a $Q$-Hermitian Hamiltonian $\hat{H}_{\text{eff}}$ after the long time development. In fact, the normalized state $|A_i(t)\rangle_N \simeq |\Lambda_i(t)\rangle_N \equiv \frac{1}{\sqrt{|\langle \Lambda_i(t)\rangle_Q \lambda_i(t)\rangle}} |\Lambda_i(t)\rangle$ and the expectation value of an operator $\mathcal{O}$, $\langle \hat{O} \rangle_Q^{\Lambda_i \Lambda_i}(t) \simeq \langle \hat{O} \rangle_Q^{\Lambda_i \Lambda_i}(t) \equiv N \langle \Lambda_i(t)\rangle_Q \langle \Lambda_i(t)\rangle_N$, obey

$$i\hbar \frac{d}{dt} \langle \Lambda_i(t)\rangle_N = \hat{H}_{\text{eff}}|\Lambda_i(t)\rangle_N,$$

$$\frac{d}{dt} \langle \hat{O} \rangle_Q^{\Lambda_i \Lambda_i}(t) = -i \frac{\hbar}{\pi} \left[ \hat{O}, \hat{H}_{\text{eff}} \right] |\Lambda_i(t)\rangle_Q.$$  

Thus we have seen for pure states that the $Q$-hermitian Hamiltonian $\hat{H}_{\text{eff}}$ emerges.

3. Density matrices for mixed states in the future-not-included CAT

In this section we define density matrices to describe mixed states and study the automatic hermiticity mechanism for them in the future-not-included CAT. For a given ensemble $6 \{|A_i(t)\rangle\}$, each of which obeys Eq. (1), let us consider a mixed state that is composed of $|A_i(t)\rangle_N$ with the probability $q_i$ for each index $i$ ($q_i \geq 0, \sum_i q_i = 1$). We define the density matrix $7$ and expectation value of an operator $\hat{O}$ for it by

$$\rho_Q^{A_i A_j}(t) = \sum_i q_i |A_i(t)\rangle_N \langle A_i(t)\rangle_Q \equiv \sum_i q_i \rho_Q^{A_i A_i}(t),$$

$$\langle \hat{O} \rangle_Q^{A_i A_j}(t) = \text{tr} \left( \rho_Q^{A_i A_j}(t) \hat{O} \right) \equiv \sum_i q_i \langle \hat{O} \rangle_Q^{A_i A_i}(t) = \sum_i q_i \langle \hat{O} \rangle_Q^{A_i A_i}(t).$$

$6$We note that each $|A_i(t)\rangle$ does not need to be orthogonal to each other, and that the number of elements does not have to match the order of the Hilbert space.

$7$When the density matrix is composed of only one component, $\rho_Q^{A_i A_j}(t) = |A_1(t)\rangle_N \langle A_1(t)\rangle_Q$, it describes a pure state, and satisfies $\rho_Q^{A_i A_j}(t)^2 = \rho_Q^{A_i A_j}(t)$ and $\text{tr} \left( \rho_Q^{A_i A_j}(t) \right) = 1$. 

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where \( \hat{\rho}_Q^{A,A}(t) \) obeys \( \hat{\rho}_Q^{A,A}(t)^2 = \hat{\rho}_Q^{A,A}(t) \) and \( \text{tr}(\hat{\rho}_Q^{A,A}(t)) = 1 \). We note that \( \hat{\rho}_Q^{A,A}(t) \) and \( \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \) are \( Q \)-Hermitian and real for \( Q \)-Hermitian \( \hat{Q} \), respectively. They time-develop as follows:

\[
\frac{d}{dt} \hat{\rho}_Q^{A,A}(t) = -\frac{i}{\hbar} \left[ \hat{H}_{Qh}, \hat{\rho}_Q^{A,A}(t) \right] - \frac{i}{\hbar} \sum_i q_i \left\{ \hat{\Delta} (\hat{H}_{Qh}; |A_i(t)\rangle_N), \hat{\rho}_Q^{A,A}(t) \right\} (t),
\]

\[
\frac{d}{dt} \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} = -\frac{i}{\hbar} \left[ \hat{\Delta} (\hat{H}_{Qh}; |A_i(t)\rangle_N), \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \right] (t).
\]

It is interesting that, in the classical limit, since \( \{ \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \} \) is suppressed, Ehrenfest’s theorem holds. Now, let us consider the long time development. Then, since \( |A_i(t)\rangle_N \approx |A_i(t)\rangle_N \) obeys Eq. (3), we obtain the following relations for \( \hat{\rho}_Q^{A,A}(t) \approx \hat{\rho}_Q^{A,A}(t), \hat{\rho}_Q^{A,A}(t) \approx \hat{\rho}_Q^{A,A}(t), \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \approx \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)}, \) and \( \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \approx \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \):

\[
\hat{\rho}_Q^{A,A}(t) \approx \sum_i q_i \hat{\rho}_Q^{A,A}(t) = \hat{U}_{\text{eff}}(t - T_A) \hat{\rho}_Q^{A,A}(T_A) \hat{U}_{\text{eff}}(t - T_A),
\]

\[
\langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \approx \text{tr}(\hat{\rho}_Q^{A,A}(t) \hat{O}) = \sum_i q_i \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \approx \sum_i q_i \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)}.
\]

\[
\frac{d}{dt} \hat{\rho}_Q^{A,A}(t) = -\frac{i}{\hbar} \left[ \hat{H}_{\text{eff}}, \hat{\rho}_Q^{A,A}(t) \right],
\]

\[
\frac{d}{dt} \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} = -\frac{i}{\hbar} \left[ \hat{\Delta} (\hat{H}_{\text{eff}}), \langle \hat{O} \rangle_{\hat{\rho}_Q^{A,A}(t)} \right].
\]

where \( \hat{U}_{\text{eff}}(t - T_A) \approx e^{-\frac{i}{\hbar} \hat{H}_{\text{eff}}(t - T_A)} \) is “\( Q \)-unitary”, i.e., \( U_{\text{eff}}(t - T_A)^{\dagger} = U_{\text{eff}}(t - T_A)^{-1} \). We find that \( \hat{\rho}_Q^{A,A}(t) \) obeys the von Neumann equation with the \( Q \)-Hermitian Hamiltonian \( \hat{H}_{\text{eff}} \) and Ehrenfest’s theorem holds. Thus we have confirmed that the automatic hermiticity mechanism works for mixed states as well as for pure states in the future-not-included CAT.

### 4. Density matrices for mixed states in the future-included CAT

In this section we attempt to introduce density matrices to describe mixed states and study their properties in the future-included CAT. In addition we investigate the automatic hermiticity mechanism for the mixed states. The future-included theory is described not only by the state vector \( |A_i(t)\rangle \) that time-develops forward from the initial time \( T_A \) according to the Schrödinger equation (1) but also by the other one \( |B_i(t)\rangle \) that time-develops backward from the final time \( T_B \) according to the other Schrödinger equation:

\[
\frac{\hbar}{4} \frac{d}{dt} |B_i(t)\rangle = \hat{H} |B_i(t)\rangle \leftrightarrow -\frac{\hbar}{4} \frac{d}{dt} |B_i(t)\rangle = \langle B_i(t)| \hat{H} |B_i(t)\rangle \approx \langle B_i(t)| \hat{H} |B_i(t)\rangle = 1.\]

The normalized matrix element

\[
\langle \hat{O} \rangle_{Q A_i(t)} = \frac{\langle B_i(t)| \hat{O} |A_i(t)\rangle}{\langle B_i(t)|Q A_i(t)\rangle} = \frac{\langle B_i(t)|Q A_i(t)\rangle}{\langle B_i(t)|Q A_i(t)\rangle} = 1.
\]

is a good candidate for an expectation value of an operator \( \hat{O} \) in the future-included CAT, because, if it is viewed as such, then we can obtain the Heisenberg equation, Ehrenfest’s theorem, and a conserved probability current density [21,22].

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\(^8\)We adopt a convention with an index \( i \) for the state, since it will be convenient later.

\(^9\)In Ref. [23], we adopted the modified inner product \( I_Q \) for all quantities in the future-included CAT [1,21,22]. We follow this formalism in this letter.

\(^10\)In the case of \( Q = 1 \), this corresponds to the weak value [18,20] that is well known in the RAT.
In the future-included CAT, let us consider the other ensemble \( \{|B_i(t)\}\) besides the ensemble \( \{|A_i(t)\}\). Now we have a simple question: what kind of mixed states can be considered in the future-included theory? One possible candidate would be the same type of mixed states as we considered in the previous section. Since \( |A_i(t)\rangle \) time-develops according to Eq. (1) in the same way as before, let us consider the same mixed state described by the density matrix \( \hat{\rho}_{Q}^{A,A_{\text{mixed}}}(t) \) defined in Eq. (5) for \( |A_i(t)\rangle \), and consider similar ones for \( |B_i(t)\rangle \). Let us introduce a normalized state and an expectation value of an operator \( \hat{O} \) for it by \( \langle B(t)\rangle_N = \frac{1}{\sqrt{|B(t)\rangle_N \langle B(t)|}} |B(t)\rangle \) and \( \langle \hat{O} \rangle_{B,B_{\text{Q}}}(t) = \frac{d}{dt} \langle B(t)\rangle_N \langle B(t)| \hat{O} |B(t)\rangle_N \), which time-develop as 

\[
\hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) = \frac{-i}{\hbar} \left[ \hat{\rho}_{Q}^{B,B_{\text{mixed}}}, \hat{O} \right] - \hbar (\hat{H}_{Qa} | B(t)\rangle_N \langle B(t)|), \quad \frac{d}{dt} \langle \hat{O} \rangle_{B,B_{\text{mixed}}}(t) = \frac{-i}{\hbar} \left[ \hat{\rho}_{Q}^{B,B_{\text{mixed}}}, \hat{O} \right].
\]

Next let us consider a mixed state that is given by \( |B(t)\rangle_N \) with the probability \( r_i \) for each index \( i \) \( (r_i \geq 0, \sum_i r_i = 1) \). We define the density matrix to describe the mixed state and the expectation value of \( \hat{O} \) for it by \( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) = \sum_i r_i |B_i(t)\rangle_N \langle B_i(t)| \hat{O} |B_i(t)\rangle_N \langle B_i(t)| \hat{O} |B_i(t)\rangle_N \langle B_i(t)|, \quad \langle \hat{O} \rangle_{B,B_{\text{mixed}}}(t) = \text{tr} \left( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \hat{O} \right) \equiv \sum_i r_i \left( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \right) |B_i(t)\rangle_N \langle B_i(t)| \hat{O} |B_i(t)\rangle_N \langle B_i(t)| \hat{O} |B_i(t)\rangle_N \langle B_i(t)|, \quad \text{tr} \left( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \right) = 1, \quad \text{tr} \left( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \right) = 1. \]

We note that \( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \) and \( \langle \hat{O} \rangle_{B,B_{\text{mixed}}}(t) \) are \( Q \)-Hermitian and real for \( Q \)-Hermitian \( \hat{O} \). They time-develop as follows: 

\[
\frac{d}{dt} \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) = -\frac{i}{\hbar} \left[ \hat{\rho}_{Q}^{B,B_{\text{mixed}}}, \hat{O} \right] + \frac{1}{\hbar} \sum_i r_i \left( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}, \hat{H}_{Qa} | B(t)\rangle_N \langle B(t)| \hat{O} |B(t)\rangle_N \langle B(t)| \hat{O} |B(t)\rangle_N \langle B(t)| \right) \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t),
\]

for each index \( i \). The only difference is that the sign in front of \( \hat{H}_{Qa} \) is opposite. Therefore, if we use the automatic hermiticity mechanism for \( |B(t)\rangle = \sum_j b_j(t) |\lambda_j\rangle \), then obtaining 

\[
|B(t)\rangle \sim e^{\frac{i}{\hbar} (T_B - t) \hat{H}_{\text{eff}}(t) \hat{B}(t) |B(t)\rangle} \equiv \sum_j b_j(t) |\lambda_j\rangle \equiv |\tilde{B}(t)\rangle \quad \text{for large } T_B - t,
\]

we find that the relations for \( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \) become the same as those for \( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \). Thus we have seen that the automatic hermiticity mechanism works for mixed states described by the density matrices \( \hat{\rho}_{Q}^{A,A_{\text{mixed}}}(t) \sim \hat{\rho}_{Q}^{A,A_{\text{mixed}}}(t) \) and \( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \), and that, via the mechanism, both of the density matrices nicely obey the von Neumann equation with the effectively obtained \( Q \)-Hermitian Hamiltonian \( \hat{H}_{\text{eff}} \). In addition, \( \hat{\rho}_{Q}^{A,A_{\text{mixed}}}(t) \) and \( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \) have real meanings as density matrices of \( |A_i(t)\rangle_N \) and \( |B_i(t)\rangle_N \). However, neither \( \text{tr} \left( \hat{\rho}_{Q}^{A,A_{\text{mixed}}}(t) \hat{O} \right) = N \langle A_i(t)| \hat{O} |A_i(t)\rangle \) nor \( \text{tr} \left( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \hat{O} \right) = N \langle B_i(t)| \hat{O} |B_i(t)\rangle \) matches the normalized matrix element \( \langle \hat{O} \rangle_{Q}^{B,A}(t) \) given in Eq. (11). In the future-included CAT, we have a philosophy such that it is not \( N \langle A_i(t)| \hat{O} |A_i(t)\rangle \) nor \( N \langle B_i(t)| \hat{O} |B_i(t)\rangle \) but \( \langle \hat{O} \rangle_{Q}^{B,A}(t) \) that has a role of an expectation value of \( \hat{O} \). Therefore, \( \hat{\rho}_{Q}^{A,A_{\text{mixed}}}(t) \) and \( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) \) might not be good density matrices in this sense. Then what should we adopt as a density matrix in the future-included CAT if we wish to respect the philosophy?

We are now motivated to consider the other kind of density matrix such that the trace of the product of each component with an index \( i \) and \( \hat{O} \) corresponds to \( \langle \hat{O} \rangle_{Q}^{B,A}(t) \). Introducing 

\[
|A_i(t)\rangle_M \equiv \frac{|A_i(t)\rangle}{\sqrt{|A_i(t)| |A_i(t)\rangle}}, \quad |B_i(t)\rangle_M \equiv \frac{|B_i(t)\rangle}{\sqrt{|B_i(t)| |B_i(t)\rangle}},
\]

which obey \( i\hbar \frac{d}{dt} |A_i(t)\rangle_M = \hat{H} |A_i(t)\rangle_M \), \( i\hbar \frac{d}{dt} |B_i(t)\rangle_M = \hat{H} |B_i(t)\rangle_M \), \( \text{tr} \left( \hat{\rho}_{Q}^{A,A_{\text{mixed}}}(t) |A_i(t)\rangle_M \langle A_i(t)| \hat{O} |A_i(t)\rangle_M \langle A_i(t)| \hat{O} |A_i(t)\rangle_M \langle A_i(t)| \hat{O} |A_i(t)\rangle_M \right) = N \langle A_i(t)| \hat{O} |A_i(t)\rangle \), \( \text{tr} \left( \hat{\rho}_{Q}^{B,B_{\text{mixed}}}(t) |B_i(t)\rangle_M \langle B_i(t)| \hat{O} |B_i(t)\rangle_M \langle B_i(t)| \hat{O} |B_i(t)\rangle_M \langle B_i(t)| \hat{O} |B_i(t)\rangle_M \right) = N \langle B_i(t)| \hat{O} |B_i(t)\rangle \).
$ih\frac{d}{dt}|B(t)\rangle_M = \tilde{H}^{Q}|B(t)\rangle_M$, and $M\langle B(t)|Q A(t)|M = 1$, let us define the following “skew density matrix” $\hat{\rho}^{B,\text{mixed}}_Q(t)$ and “expectation value” of $\hat{O}$ for it\textsuperscript{12} by

$$\rho^{B,\text{mixed}}_Q(t) \equiv \sum_i s_i|A_i(t)\rangle_M \langle B_i(t)|_Q \equiv \sum_i s_i \rho^{B,A}_Q(t),$$

$$\langle \hat{O} \rangle_{\hat{\rho}^{B,\text{mixed}}_Q(t)} = \text{tr} \left( \hat{\rho}^{B,\text{mixed}}_Q(t) \hat{\mathcal{O}} \right) \equiv \sum_i s_i \langle \hat{O} \rangle_{\rho^{B,A}_Q(t)} = \sum_i s_i \langle \hat{O} \rangle_{\hat{\rho}^{B,A}_Q(t)},$$

where the weight $s_i$ for each $\rho^{B,A}_Q(t)$ obeys $s_i \geq 0$, $\sum s_i = 1$, and $\rho^{B,A}_Q(t)$ obeys $\text{tr} (\rho^{B,A}_Q(t)) = 1$. Therefore, $\rho^{B,\text{mixed}}_Q(t)$ can be expressed as $\rho^{B,\text{mixed}}_Q(t) = \hat{U}(t-t_f) \rho^{B,\text{mixed}}_Q(t_f) \hat{U}(t-t_f)^{-1}$, where $\hat{U}(t-t_f) \equiv e^{-\frac{i}{\hbar} \tilde{H}(t-t_f)}$ is neither unitary nor $Q$-unitary, and $t_f$ is a reference time. They time-develop as follows:

$$\frac{d}{dt} \rho^{B,\text{mixed}}_Q(t) = -\frac{i}{\hbar} \left[ \tilde{H}, \rho^{B,\text{mixed}}_Q(t) \right],$$

which show that $\rho^{B,\text{mixed}}_Q(t)$ obeys the von Neumann equation and Ehrenfest’s theorem holds as they are. These properties are quite in contrast to those of $\rho^{A,A}_{Q,\text{mixed}}(t)$ and $\rho^{B,B}_{Q,\text{mixed}}(t)$. If we consider the long time development, then for $|A_i(t)\rangle_M \simeq |\tilde{A}_i(t)\rangle_M = \frac{|\tilde{A}_i(t)\rangle}{\sqrt{|\tilde{A}_i(t)\rangle_M \langle \tilde{A}_i(t)|M}}$ and $|B_i(t)\rangle_M \simeq |\tilde{B}_i(t)\rangle_M = \frac{|\tilde{B}_i(t)\rangle}{\sqrt{|\tilde{B}_i(t)\rangle_M \langle \tilde{B}_i(t)|M}}$, we find that $\rho^{B,\text{mixed}}_Q(t) \simeq \rho^{B,\text{mixed}}_Q(t_f) \equiv \sum_i s_i |\tilde{A}_i(t_f)\rangle_M \langle \tilde{B}_i(t_f)|_Q \equiv \sum_i s_i p^{B,\text{mixed}}_Q(t_f)$, and

$$\langle \hat{O} \rangle_{\rho^{B,\text{mixed}}_Q(t) \simeq \langle \hat{O} \rangle_{\rho^{B,\text{mixed}}_Q(t_f)} \equiv \text{tr} \left( \rho^{B,\text{mixed}}_Q(t_f) \hat{\mathcal{O}} \right) \equiv \sum_i s_i \langle \hat{O} \rangle_{\rho^{B,\text{mixed}}_Q(t_f)} = \sum_i s_i \langle \hat{O} \rangle_{\rho^{B,\text{mixed}}_Q(t_f)}$$

time-develop with an effectively obtained $Q$-Hermitian Hamiltonian $\tilde{H}_{\text{eff}}$ as follows:

$$\frac{d}{dt} \rho^{B,\text{mixed}}_Q(t) = -\frac{i}{\hbar} \left[ \tilde{H}_{\text{eff}}, \rho^{B,\text{mixed}}_Q(t) \right].$$

However, $\rho^{B,\text{mixed}}_Q(t)$ and $\langle \hat{O} \rangle_{\rho^{B,\text{mixed}}_Q(t)}$ are neither $Q$-Hermitian nor real for $Q$-Hermitian $\hat{O}$, respectively, because $|\tilde{A}_i(t)\rangle_M$ and $|\tilde{B}_i(t)\rangle_M$ are different states. This is quite in contrast to the cases for $\rho^{A,A}_{Q,\text{mixed}}(t)$ and $\rho^{B,B}_{Q,\text{mixed}}(t)$, where only either $|A_i(t)\rangle_N$ or $|B_i(t)\rangle_N$ is used. To resolve this problem, we will consider it in another way.

5. Hermiticity and reality for $\hat{\rho}^{B,\text{mixed}}_Q(t)$ and $\langle \hat{O} \rangle_{\rho^{B,A,\text{mixed}}_Q(t)}$

In Ref. [21], utilizing the automatic hermiticity mechanism for pure states time-developing forward and backward, we obtained the following correspondence:

$$\langle \mathcal{O} \rangle^{B,A}_Q$$

for large $T_B - t$ and large $t - T_A \simeq \langle \mathcal{O} \rangle^{A,A}_Q$$

for large $t - T_A$, \textsuperscript{14} based on the Schrödinger equations (1) and $ih\frac{d}{dt}|B(t)\rangle = \hat{H}|B(t)\rangle$, where $\langle \mathcal{O} \rangle^{B,A}_Q = \frac{|\langle B(t)\rangle_{Q,A(t)}\rangle}{|\langle B(t)\rangle_{Q,A(t)}\rangle}$ is a matrix element of an operator $\mathcal{O}$ defined with a usual inner product (Q = 1) in the future-included theory, while $\langle \mathcal{O} \rangle^{A,A}_Q = \frac{|\langle A(t)\rangle_{Q,A(t)}\rangle}{|\langle A(t)\rangle_{Q,A(t)}\rangle}$ is a usual expectation value of $\mathcal{O}$ defined with a

\textsuperscript{12} $\langle \hat{O} \rangle_{\hat{\rho}^{B,\text{mixed}}_Q(t)} = \sum_i s_i \text{tr} \left( \rho^{B,A}_Q(t) \hat{O} \right) = \sum_i s_i \frac{\text{tr} \left( \hat{\rho}^{B,\text{mixed}}_{Q,\text{eff}}(t) \hat{O} \right)}{\text{tr} \left( \hat{\rho}^{B,\text{mixed}}_{Q,\text{eff}}(t) \right)}$ for $Q = 1$ corresponds to the weak value for the generalized state introduced in Ref. [19], but is different from the generalized weak value $\frac{\text{tr} \left( \hat{\rho}^{B,\text{mixed}}_{Q,\text{eff}}(t) \hat{O} \right)}{\text{tr} \left( \hat{\rho}^{B,\text{mixed}}_{Q,\text{eff}}(t) \right)}$ introduced in Refs. [34,35]. The latter expression is more general since the numbers of ensembles of initial and final states for the density matrices $\hat{\rho}_{i}$ and $\hat{\rho}_{f}$ are taken independently, while, in our skew density matrix, the numbers of ensembles are supposed to be equal. This is because we are keeping in mind the maximization principle, by which a pair of initial and final states is generically chosen such that the absolute value of the transition amplitude is maximized. Then, in a situation such that a pair $\{|A_i\}, |B_i\rangle$ and each weight $\{s_i\}$ are given, our skew density matrix enables us to calculate and simulate the “expectation value” of $\hat{O}$.
modified inner product $I_Q$ in the future-not-included theory. We showed this correspondence by improving the method used in Ref. [1], which first multiplies $\langle O \rangle^\text{BA}_Q$ by $1 = \frac{(A(t))|B(t))}{(A(t))|B(t))}$ and then evaluates $|B(t)\rangle\langle B(t)|$. This correspondence strongly suggests that the future-included CAT is not excluded phenomenologically, even though it looks very exotic. Utilizing this method, let us estimate $\langle O \rangle^\text{BA}_Q$ and $\hat{p}^\text{BA}_Q(t)$, based on the Schrödinger equations (1) and $ih\frac{d}{dt}|B(t)\rangle = \hat{H}^1|B(t)\rangle$. Respecting the inner product $I_Q$ for all quantities, let us multiply $\langle O \rangle^\text{BA}_Q(t)$ by $1 = \frac{(A(t))|O B(t))}{(A(t))|O B(t))}$, instead of $1 = \frac{(A(t))|B(t))}{(A(t))|O B(t))}$. Then $\langle O \rangle^\text{BA}_Q(t)$ is rewritten as $\langle O \rangle^\text{BA}_Q(t) = \frac{(A(t))|O B(t))}{(A(t))|O B(t))}$ $\frac{(A(t))|B(t))}{(A(t))|O B(t))}$. The expansion of $|B(T_B)\rangle$ used in Ref. [21], $|B(T_B)\rangle = \sum |\lambda_i\rangle_B$ in terms of the eigenstate of $\hat{H}^1$, $|\lambda_B = Q|\lambda_i\rangle$, is found to produce too many $Q$, so it does not seem to be an appropriate choice in the present study. Hence we adopt another expansion: $|B(T_B)\rangle = \sum |\lambda_i\rangle_B = \sum J(\lambda_i)^*|\lambda_i\rangle$, where $J(\lambda_i)$ is a function of $\lambda_i$. Then $|B(t)\rangle\langle B(t)|Q$ is evaluated as follows:

$$
|B(t)\rangle\langle B(t)|Q = e^{-i\hat{H}^\text{BA}(t-T_B)}|B(T_B)\rangle\langle B(T_B)|Q e^{i\hat{H}^\text{BA}(t-T_B)} = \sum_{i,j} c_i c_j^* e^{i\text{Re}(\lambda_j - \lambda_i)(t-T_B)} e^{i\text{Im}(\lambda_j + \lambda_i)(t-T_B)}|\lambda_j\rangle_i \langle \lambda_j|Q
$$

$$
|B(t)\rangle\langle B(t)|Q \approx \frac{\int_{t-\Delta t}^{t+\Delta t} |B(t)\rangle\langle B(t)|Q dt}{\int_{t-\Delta t}^{t+\Delta t} dt} \approx \sum_{i} |c_i|^2 e^{i\text{Im}(\lambda_i)^{-1}/2}\langle \lambda_i|Q
$$

$$
\approx e^{i\hat{H}^\text{BA}(t-T_B)}Q_4 \quad \text{for large } T_B - t,
$$

where in the third line we have smeared the present time $t$ a little bit, and the off-diagonal elements wash to 0. In the last line we have used the automatic hermiticity mechanism for large $T_B - t$, and introduced $Q_4 = \sum_{\lambda_i} |c_i|^2|\lambda_i\rangle\langle \lambda_i|Q$, which is expressed as follows:

$$
Q_4 = J(\hat{H}_\text{eff} + iBA\Lambda)\|^0\Lambda_A J(\hat{H}_\text{eff} + iBA\Lambda) = Q^{-1}J(\hat{H}_\text{eff})^\dagger Q(J\hat{H}_\text{eff}) = Q^{-1}Q_J.\text{ Here, supposing that } \text{Re}\lambda_i \text{ are not degenerate, we have introduced } \Lambda_A = \sum_{\lambda_i} |\lambda_i\rangle\langle \lambda_i|Q, \text{ a function } J \text{ such that } J(\text{Re}\lambda_i) = J(\text{Re}\lambda_i + iB) = c_i^* \text{ for } i \in A, \text{ and } Q_J = J(\hat{H}_\text{eff})^\dagger Q(J\hat{H}_\text{eff}). \text{ Now we use the automatic hermiticity mechanism for large } t - T_A. \text{ Then, since } |A(t)\rangle = \sum_{\lambda_i} a_i(t)|\lambda_i\rangle \text{ behaves as } |\hat{A}(t)\rangle = \sum_{\lambda_i} a_i(t)|\lambda_i\rangle, \text{ we obtain } \langle O \rangle^\text{BA}_Q \approx \langle \hat{A}(t)|O\rangle^{\hat{A}(t)} = \langle O \rangle^\text{BA}_J \text{ for large } T_B - t \text{ and large } t - T_A.
$$

Next, let us consider the expectation value in the future-not-included theory: $\langle O \rangle^\text{AA}_Q = \frac{(A(t))|O B(t))}{(A(t))|O B(t))}$, where $Q_J \equiv J(\hat{H}_\text{eff})^\dagger Q(J\hat{H}_\text{eff}) = (P_{J-1})^{-1}P_{J-1}^{-1}$, and $P_{J-1} \equiv J(\hat{H})^{-1}$ $P$ diagonalizes $\hat{H}: (P_{J-1})^{-1}\hat{H}P_{J-1} = P^{-1}\hat{H}P = D$. We introduce $|\lambda_i\rangle^{J-1} = J(\hat{H})^{-1}|\lambda_i\rangle$, so that $|\lambda_i\rangle^{J-1}$ is $Q_J$-orthogonal, i.e., $I_Q(|\lambda_i\rangle^{J-1}, |\lambda_j\rangle^{J-1}) = \delta_{ij}$. We use the automatic hermiticity mechanism for large $t - T_A$. $|A(t)\rangle$ behaves as $|\hat{A}(t)\rangle = \sum_{\lambda_i} a_i(t)|\lambda_i\rangle$, and $Q_J$ is estimated as follows: $Q_J \approx J(\hat{H}_\text{eff} + iBA\Lambda)Q(J\hat{H}_\text{eff} + iBA\Lambda) = J(\hat{H}_\text{eff})^\dagger Q(J\hat{H}_\text{eff}) = Q_J$. Then the expectation value in the future-not-included theory is expressed as $\langle O \rangle^\text{AA}_Q \approx \langle \hat{A}(t)|O\rangle^{\hat{A}(t)} = \langle O \rangle^\text{AA}_J$ for large $t - T_A$. Thus we have obtained the following correspondence:

$$
\langle O \rangle^\text{BA}_Q \text{ for large } T_B - t \text{ and large } t - T_A \approx \langle O \rangle^\text{AA}_J \approx \langle O \rangle^\text{AA}_Q \text{ for large } t - T_A,
$$

which suggests that the future-included theory is not excluded, although it looks very exotic. $\langle O \rangle^\text{BA}_J$ is real for $Q_J$-Hermitian $O$, and time-develops according to the $Q_J$-Hermitian Hamiltonian $\hat{H}_\text{eff}$. We can apply this correspondence to each $i$-component $\langle \check{O} \rangle^\text{AA}_i(t)$.
Next let us evaluate the skew density matrix $\hat{\rho}_Q^{BA}(t) = \frac{\langle B(t)|A(t) \rangle}{\langle A(t)|B(t) \rangle}$ by multiplying it by $1 = \frac{\langle A(t) | Q(t) \rangle}{\langle Q(t) | A(t) \rangle}$. Utilizing the above evaluation of $\langle B(t)|A(t) \rangle_Q$, we obtain the correspondence:

$$
\hat{\rho}_Q^{BA}(t) = \hat{\rho}_Q^{\hat{A}\hat{A}}(t) \propto \hat{\rho}_Q^{\hat{A}\hat{A}}(t) \propto \hat{\rho}_Q^{\hat{A}\hat{A}}(t)
$$

where $\hat{\rho}_Q^{\hat{A}\hat{A}}(t) = \frac{\langle A(t) | \hat{A}(t) \rangle_{Q(t)}}{\langle A(t) | Q(t) \rangle_{Q(t)}}$.

Here $t_r$ is a reference time, and $\hat{\rho}_Q^{\hat{A}\hat{A}}(t)$ obeys $\text{tr}(\hat{\rho}_Q^{\hat{A}\hat{A}}(t)) = 1$ and $\hat{\rho}_Q^{\hat{A}\hat{A}}(t) = \hat{\rho}_Q^{\hat{A}\hat{A}}(t)$. $\hat{U}_{\text{eff}}(t - t_r)$ is $Q_f$-unitary, and $\hat{\rho}_Q^{\hat{A}\hat{A}}(t)$ is $Q_f$-Hermitian. We can apply this correspondence to each $i$-component $\hat{\rho}_Q^{BA_i}(t)$ as

$$
\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA_i}(t)} = \text{tr}(\hat{\rho}_Q^{BA_i}(t)\hat{O}) \propto \text{tr}(\hat{\rho}_Q^{\hat{A}\hat{A}}(t)\hat{O}) \equiv \langle \hat{O} \rangle_{\hat{\rho}_Q^{\hat{A}\hat{A}}(t)}
$$

which is real for $Q_f$-Hermitian $\hat{O}$. Finally,

$$
\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA_i}(t)} \propto \hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t) = \sum_i s_i \hat{\rho}_Q^{\hat{A}\hat{A}}(t)
$$

and

$$
\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA_i}(t)} \propto \hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t) = \sum_i s_i \langle \hat{O} \rangle_{\hat{\rho}_Q^{\hat{A}\hat{A}}(t)}
$$

time-develop according to

$$
\frac{d}{dt} \hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t) = -\frac{i}{\hbar} \left[ \hat{H}_{\text{eff}}, \hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t) \right],
$$

$$
\frac{d}{dt} \langle \hat{O} \rangle_{\hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t)} = -\frac{i}{\hbar} \left[ \langle \hat{O} \rangle, \hat{H}_{\text{eff}} \right]_{\hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t)}
$$

which show that $\hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t)$ obeys the von Neumann equation with the $Q_f$-Hermitian Hamiltonian $\hat{H}_{\text{eff}}$ and Ehrenfest’s theorem holds. We note that $\hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t)$ is $Q_f$-Hermitian, and $\langle \hat{O} \rangle_{\hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t)}$ is real for $Q_f$-Hermitian $\hat{O}$. Thus we have seen that the problem with $\hat{\rho}_Q^{BA_i}(t)$ and $\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA_i}(t)}$ mentioned at the end of the previous section can be effectively resolved by considering the long time development for large $T_B - t$ and large $t - T_A$.

6. Discussion

We first reviewed the modified inner product $I_Q$ that makes a given non-normal Hamiltonian normal with regard to it, and the automatic hermiticity mechanism [13,14,21], which we previously proposed and studied for pure states in the CAT. Next, in the case of the future-not-included CAT, we defined a density matrix $\hat{\rho}_Q^{\hat{A}\hat{A},\text{mixed}}(t)$ to describe a mixed state and an expectation value of an operator $\hat{O}$ for it, and studied their properties. In the classical limit, $\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA_i}(t)}$ time-develops by a $Q$-Hermitian Hamiltonian, and Ehrenfest’s theorem holds. In addition, we showed that, if we consider a long time development, eigenvectors having the largest imaginary part of the eigenvalues of $\hat{H}$ dominate most. On the subspace spanned by such eigenvectors, a $Q$-Hermitian Hamiltonian effectively emerges, the expectation value of $\hat{O}$ becomes real for $Q$-Hermitian $\hat{O}$, and the density matrix obeys the von Neumann equation with the $Q$-Hermitian
Hamiltonian. Thus we confirmed that the automatic hermiticity mechanism works for mixed states in the future-not-included theory.

The situation becomes more non-trivial in the future-included theory, because, in the future-included theory, there are two classes of ensembles of state vectors, \(\{|A_i(t)\rangle\}\) and \(\{|B_i(t)\rangle\}\), that time-develop forward from the initial time \(T_A\) and backward from the final time \(T_B\), respectively. So it seems that there are at least a couple of candidates for density matrices in the future-included theory. As the first candidate, we investigated a pair of density matrices \(\hat{\rho}^{AA,\text{mixed}}_Q(t)\) and \(\hat{\rho}^{BB,\text{mixed}}_Q(t)\), which are composed of only either \(\{|A_i(t)\rangle\}\) or \(\{|B_i(t)\rangle\}\), and argued that, though the pair has nice properties, it has a common disadvantage in the future-included theory. In general, the trace of the product of a density matrix and an operator \(O\) has to match an expectation value of \(O\), but this is not the case for this pair, because it is the matrix element of \(O, \langle O \rangle^{BA}_Q\), that is expected to work as an expectation value of \(O\) in the future-included theory. To resolve this problem, we introduced a “skew density matrix” \(\hat{\rho}^{BA,\text{mixed}}_Q(t)\), which is composed of both \(\{|A_i(t)\rangle\}\) and \(\{|B_i(t)\rangle\}\). The skew density matrix has a nice property such that the trace of the product of it and an operator \(O\) matches the matrix element \(\langle O \rangle^{BA}_Q(t)\). It also obeys the von Neumann equation as it is. In addition, utilizing the automatic hermiticity mechanism, we showed that the skew density matrix \(\hat{\rho}^{BA,\text{mixed}}_Q(t)\) and matrix element \(\langle O \rangle^{BA}_Q(t)\) defined with an inner product \(I_Q\) in the future-included theory for large \(T_B - t\) and large \(t - T_A\) approximately correspond to another density matrix \(\hat{\rho}^{AA,\text{mixed}}_Q(t)\) and an expectation value \(\langle O \rangle^{AA}_Q(t)\) defined with another inner product \(I_Q\) in the future-not-included theory for large \(t - T_A\). Therefore, even though the skew density matrix is not a density matrix in a usual sense, it can effectively work as if it were a usual density matrix. Thus we argued that it is the skew density matrix that is expected to have a role of a density matrix in the future-included theory. In addition, we confirmed that the automatic hermiticity mechanism works for mixed states in the future-included theory.

Now density matrices have been implemented in the CAT. What should we study by using them? It would be interesting to investigate the classical dynamics of the CAT in phase space via the Wigner function. For this purpose, it would be better to study further in detail the harmonic oscillator model that we previously formulated by introducing the two-basis formalism [36]. Also, it would be intriguing to evaluate von Neumann entropy in the CAT. Furthermore, density matrices are necessary tools if we wish to investigate quantum measurement quantitatively in a composite system via the master equation. We would like to report such studies in the future.

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References

[1] H. B. Nielsen and M. Ninomiya, Proc. Bled 2006: What Comes Beyond the Standard Models, p. 87 (2006) [arXiv:hep-ph/0612250] [Search inSPIRE].
[2] H. B. Nielsen and M. Ninomiya, Int. J. Mod. Phys. A 23, 919 (2008).
[3] H. B. Nielsen and M. Ninomiya, Int. J. Mod. Phys. A 24, 3945 (2009).
[4] H. B. Nielsen and M. Ninomiya, Prog. Theor. Phys. 116, 851 (2007).
[5] H. B. Nielsen and M. Ninomiya, Proc. Bled 2007: What Comes Beyond the Standard Models, p. 144 (2007) [arXiv:0711.3080 [hep-ph]] [Search inSPIRE].
[6] H. B. Nielsen and M. Ninomiya, arXiv:0910.0359 [hep-ph] [Search inSPIRE].
[7] H. B. Nielsen, Found. Phys. 41, 608 (2011) [arXiv:0911.4005 [quant-ph]] [Search inSPIRE].
[8] H. B. Nielsen and M. Ninomiya, Proc. Bled 2010: What Comes Beyond the Standard Models, p. 138 (2010) [arXiv:1008.0464 [physics.gen-ph]] [Search inSPIRE].
[9] H. B. Nielsen, arXiv:1006.2455 [physics.gen-ph] [Search inSPIRE].
[10] H. B. Nielsen and M. Ninomiya, arXiv:hep-th/0701018 [Search inSPIRE].
[11] H. B. Nielsen, Found. Phys. 41, 608 (2011) [arXiv:0911.4005 [quant-ph]] [Search inSPIRE].
[12] H. B. Nielsen and M. Ninomiya, arXiv:0910.0359 [hep-ph] [Search inSPIRE].
[13] H. B. Nielsen and M. Ninomiya, Prog. Theor. Phys. 125, 633 (2011).
[14] K. Nagao and H. B. Nielsen, Prog. Theor. Phys. 126, 1021 (2011); 127, 1131 (2012) [erratum].
[15] K. Nagao and H. B. Nielsen, Int. J. Mod. Phys. A 27, 1250076 (2012); 32, 1792003 (2017) [erratum].
[16] K. Nagao and H. B. Nielsen, Prog. Theor. Exp. Phys. 2013, 073A03 (2013); 2018, 029201 (2018) [erratum].
[17] K. Nagao and H. B. Nielsen, Prog. Theor. Exp. Phys. 2017, 111B01 (2017).
[18] Y. Aharonov, D. Z. Albert, and L. Vaidman, Phys. Rev. Lett. 60, 1351 (1988).
[19] Y. Aharonov and L. Vaidman, J. Phys. A. Math. Gen. 24, 2315 (1991).
[20] Y. Aharonov, S. Popescu, and J. Tollaksen, Phys. Today 63, 27 (2010).
[21] K. Nagao and H. B. Nielsen, Prog. Theor. Exp. Phys. 2013, 023B04 (2013); 2018, 039201 (2018) [erratum].
[22] K. Nagao and H. B. Nielsen, Proc. Bled 2012: What Comes Beyond the Standard Models, p. 86 (2012) [arXiv:1211.7269 [quant-ph]] [Search inSPIRE].
[23] K. Nagao and H. B. Nielsen, Prog. Theor. Exp. Phys. 2015, 051B01 (2015).
[24] K. Nagao and H. B. Nielsen, Prog. Theor. Exp. Phys. 2017, 081B01 (2017).
[25] C. M. Bender and S. Boettcher, Phys. Rev. Lett. 80, 5243 (1998).
[26] C. M. Bender, S. Boettcher, and P. Meisinger, J. Math. Phys. 40, 2201 (1999).
[27] A. Mostafazadeh, J. Math. Phys. 43, 3944 (2002).
[28] A. Mostafazadeh, J. Math. Phys. 44, 974 (2003).
[29] C. M. Bender and P. D. Mannheim, Phys. Rev. D 84, 105038 (2011).
[30] K. Nagao and H. B. Nielsen, Fundamentals of Quantum Complex Action Theory (Lambert, Saarbrücken, 2017).
[31] K. Nagao and H. B. Nielsen, Proc. Bled 2017: What Comes Beyond the Standard Models, p. 121 (2017) [arXiv:1710.02071 [quant-ph]] [Search inSPIRE].
[32] K. Nagao and H. B. Nielsen, Prog. Theor. Exp. Phys. 2022, 091B01 (2022).
[33] F. G. Scholtz, H. B. Geyer, and F. J. W. Hahne, Ann. Phys. 213, 74 (1992).
[34] S. Wu and K. Mølmer, Phys. Lett. A 374, 34 (2009).
[35] S. Tamate, T. Nakamishi, and M. Kitano, arXiv:1211.4292 [quant-ph] [Search inSPIRE].
[36] K. Nagao and H. B. Nielsen, Prog. Theor. Exp. Phys. 2019, 073B01 (2019).