Automatic hermiticity for mixed states

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Based on the work with Holger Bech Nielsen, PTEP (2023) 031B01

Introduction

H.B.Nielsen, M.Ninomiya, Proc. Bled 2006, p.87

Complex action theory (CAT) \leftarrow Extension of quantum theory

- coupling parameters are complex
- in Feynman path integral, measure is path-dependent.
- corresponding Hamiltonian is non-normal.
 * PT symmetric Hamiltonian : Bender and Boettcher etc.

It would be nice if we could remove a constraint of an action being real. \leftarrow One of the benefits Less constraints, more fundamental.

Expected to give natural initial states \Leftarrow One of the benefits \Rightarrow Falsifiable predictions have been intensively studied by H. B. Nielsen and M. Ninomiya

Four types of quantum theory

Quantum theory can be classified into four types, according to whether its action is real or not, and whether the future is included or not.

	Real action	Complex action
Future not included	FNI RAT	FNI CAT
Future included	FI RAT	FI CAT

 Table: Four types of quantum theory.

* Complex action suggests future-included theory

KN and H.B.Nielsen, PTEP 2017 111B01

The future-not-included theory

Usual quantum theory is defined with a given past state $|A(T_A)\rangle$ at the initial time T_A , which time-develops forward as

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

The expectation value of \hat{O} is given by $\langle \hat{O} \rangle^{AA} = \frac{\langle A(t) | \hat{O} | A(t) \rangle}{\langle A(t) | A(t) \rangle}$.

* Eat right, future bright.

 \Rightarrow We call this theory "future-not-included" theory.

The future-included theory

H.B.Nielsen, M.Ninomiya, Proc. Bled 2006, p.87

We can consider another theory, "future-included" theory, in which not only a past state $|A(T_A)\rangle$ at the initial time T_A , but also a future state $|B(T_B)\rangle$ at the final time T_B is given:

$$i\hbar \frac{d}{dt}|A(t)\rangle = \hat{H}|A(t)\rangle, \quad -i\hbar \frac{d}{dt}\langle B(t)| = \langle B(t)|\hat{H},$$

where \hat{H} is non-normal.

The normalized matrix element $\langle \hat{O} \rangle^{BA} \equiv \frac{\langle B(t)|\hat{O}|A(t)\rangle}{\langle B(t)|A(t)\rangle}$ is expected to work as an "expectation value" of \hat{O} .

* $\langle \hat{O} \rangle^{BA}$ is called the weak value in the real action theory (RAT).

Y. Aharonov, D. Z. Albert, L. Vaidman, Phys. Rev. Lett. 60 (1988) pp.1351-1354

KN, H.B.Nielsen, PTEP 2013 023B04

If we regard $\langle \hat{O} \rangle^{BA}$ as an expectation value in the future-included theory, then, utilizing $\frac{d}{dt} \langle O \rangle^{BA} = \langle \frac{i}{\hbar} [\hat{H}, O] \rangle^{BA}$, we obtain

- Heisenberg equation
- Ehrenfest's theorem:

$$\frac{d}{dt} \langle \hat{q}_{new} \rangle^{BA} = \frac{1}{m} \langle \hat{p}_{new} \rangle^{BA},$$
$$\frac{d}{dt} \langle \hat{p}_{new} \rangle^{BA} = -\langle V'(\hat{q}_{new}) \rangle^{BA}.$$

* momentum relation $p = m\dot{q}$

KN, H.B.Nielsen, IJMP **A27**(2012) 1250076;Erratum-ibid, **A32**(2017) 1792003

* complex coordinate and momentum formalism

KN, H.B.Nielsen, PTP126 (2011)102

Conserved probability current density

 $\Rightarrow \langle \hat{O} \rangle^{BA}$ seems to play the role of an expectation value in the future-included theory. However, $\langle \hat{O} \rangle^{BA}$ is complex in general.

Difference of the philosophies

 $\langle \hat{O} \rangle^{BA} \equiv \frac{\langle B(t) | \hat{O} | A(t) \rangle}{\langle B(t) | A(t) \rangle}$

	Theory of	Our theory
	Aharonov et.al.	
mainly	experiments	whole universe
interested in	in laboratories	
look at the path s.t.	small	large
$ \langle B(t) A(t)\rangle $ is		
because	amplification	less conditions,
of	of detection	natural initial states

Our philosophy:

our universe could be realized by a path (including initial and final conditions) selected from a superposition of many possible paths of our universe that are given randomly.

Modified inner product for \hat{H}

KN and H.B.Nielsen, PTP 125(2011)633

 $\hat{H}|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$

 $|\lambda_i\rangle$: eigenstates of \hat{H} , but not orthogonal in the usual inner product $I(|\lambda_i\rangle, |\lambda_j\rangle) \equiv \langle \lambda_i | \lambda_j \rangle \neq \delta_{ij}$. $\lambda_i (i = 1, ...)$: complex

$$\hat{H} = PDP^{-1},$$

where $P = (|\lambda_1\rangle, |\lambda_2\rangle, ...), D = diag(\lambda_1, \lambda_2, ...)$

Let us consider a transition from $|\lambda_i\rangle$ to $|\lambda_j\rangle$ ($i \neq j$) fast in time Δt

$$|I(|\lambda_j\rangle, \exp\left(-\frac{i}{\hbar}\hat{H}\Delta t\right)|\lambda_i\rangle)|^2 \neq 0,$$

since $\langle \lambda_i | \lambda_j \rangle \neq 0$, even though \hat{H} cannot bring the system from $|\lambda_i\rangle$ to $|\lambda_j\rangle$ ($i \neq j$). \Rightarrow Such a transition should be prohibited. We define $I_Q(|f\rangle, |i\rangle) \equiv \langle f|_Q i\rangle \equiv \langle f|Q|i\rangle$ s.t. $I_Q(|\lambda_i\rangle, |\lambda_j\rangle) = \delta_{ij}$, and impose $\langle \psi_1(t)|_Q \psi_2(t) \rangle = \langle \psi_2(t)|_Q \psi_1(t) \rangle^* \rightarrow Q^{\dagger} = Q$

Also, we define \dagger_Q for

- any operator A: $\langle \psi_2 |_Q A | \psi_1 \rangle^* = \langle \psi_1 |_Q A^{\dagger_Q} | \psi_2 \rangle \rightarrow A^{\dagger_Q} = Q^{-1} A^{\dagger} Q$
- kets and bras: $|\psi_1\rangle^{\dagger_Q} \equiv \langle \psi_1|_Q, (\langle \psi_2|_Q)^{\dagger_Q} \equiv |\psi_2\rangle$

When *A* satisfies $A^{\dagger \varrho} = A$, we call *A Q*-Hermitian. We choose *Q* as $Q = (P^{\dagger})^{-1}P^{-1}$.

* \hat{H} is *Q*-normal: $[\hat{H}, \hat{H}^{\dagger_Q}] = [\hat{H}_{Qh}, \hat{H}_{Qa}] = 0$

$$\hat{H} = \hat{H}_{Qh} + \hat{H}_{Qa}, \quad \hat{H}_{Qh} \equiv \frac{\hat{H} + \hat{H}^{\dagger \varrho}}{2}, \quad \hat{H}_{Qa} \equiv \frac{\hat{H} - \hat{H}^{\dagger \varrho}}{2}.$$

* A similar inner product is studied also in F. G. Scholtz, H. B. Geyer and F. J. W. Hahne, Ann. Phys. 213 (1992) 74, A. Mostafazadeh, J.Math.Phys.43, 3944 (2002).

Automatic hermiticity mechanism for pure states

KN and H.B.Nielsen, PTP 125(2011)633

If the anti-Hermitain part of H is bounded from above, then H effectively becomes Hermitian with

- the modified inner product
- a long time development

(Only the modes belonging to the subspace with the maximal $\mbox{Im}\lambda_i$ dominate)

Let us consider a state $|A_i(t)\rangle$, which obeys the Schrödinger eq.

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

A normalized state $|A_i(t)\rangle_N \equiv \frac{1}{\sqrt{\langle A_i(t)|_Q A_i(t)\rangle}} |A_i(t)\rangle$ and an expectation value of an operator \hat{O} , $\langle \hat{O} \rangle_Q^{A_iA_i}(t) \equiv {}_N \langle A_i(t)|_Q \hat{O} |A_i(t)\rangle_N$, obey

$$\begin{split} &i\hbar\frac{\partial}{\partial t}|A_{i}(t)\rangle_{N}=\hat{H}_{Qh}|A_{i}(t)\rangle_{N}+\hat{\Delta}\left(\hat{H}_{Qa};|A_{i}(t)\rangle_{N}\right)|A_{i}(t)\rangle_{N},\\ &\frac{d}{dt}\langle\hat{O}\rangle_{Q}^{A_{i}A_{i}}(t)=-\frac{i}{\hbar}\langle\left[\hat{O},\hat{H}_{Qh}\right]\rangle_{Q}^{A_{i}A_{i}}(t)-\frac{i}{\hbar}\langle\left\{\hat{O},\hat{\Delta}\left(\hat{H}_{Qa};|A_{i}(t)\rangle_{N}\right)\right\}\rangle_{Q}^{A_{i}A_{i}}(t),\\ &\text{where }\hat{\Delta}\left(\hat{H}_{Qa};|A_{i}(t)\rangle_{N}\right)\equiv\hat{H}_{Qa}-{}_{N}\langle A_{i}(t)|_{Q}\hat{H}_{Qa}|A_{i}(t)\rangle_{N}. \end{split}$$

It is intriguing that, in the classical limit, $\langle \hat{O} \rangle_Q^{A_i A_i}(t)$ seems to time-develop by \hat{H}_{Qh} , and Ehrenfest's theorem holds.

We will see the emergence of the *Q*-hermiticity even before considering the classical limit if we consider a long time development.

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 $|A_i(t)\rangle = Pe^{-\frac{i}{\hbar}D(t-t_0)}|A'_i(t_0)\rangle = \sum_j a_j^{(i)}(t_0)e^{\frac{1}{\hbar}(\operatorname{Im}\lambda_j - i\operatorname{Re}\lambda_j)(t-t_0)}|\lambda_j\rangle.$

Imagine that some of $\text{Im}\lambda_j$ take the maximum value *B* (the corresponding subset of $\{j\} \equiv A$)

If a long time has passed, i.e. for large $t - t_0$, the states with $\text{Im}\lambda_j|_{j \in A}$ contribute most in the sum

We introduce a diagonalized Hamiltonian \tilde{D}_R :

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

$$H_{\text{eff}} \equiv P \tilde{D}_R P^{-1} \text{ obeys } H_{\text{eff}}^{\dagger_Q} = H_{\text{eff}}, H_{\text{eff}} |\lambda_i\rangle = \text{Re}\lambda_i |\lambda_i\rangle$$

We also introduce $|\tilde{A}_i(t)\rangle \equiv \sum_{j \in A} a_j^{(i)}(t) |\lambda_j\rangle$.

Then $|A_i(t)\rangle$ is evaluated as

$$\begin{aligned} |A_i(t)\rangle &\simeq e^{\frac{1}{\hbar}B(t-t_0)}\sum_{j\in A}a_j^{(i)}(t_0)e^{-\frac{i}{\hbar}\mathsf{R}e\lambda_j(t-t_0)}|\lambda_j\rangle \\ &= e^{\frac{1}{\hbar}B(t-t_0)}e^{-\frac{i}{\hbar}\hat{H}_{\mathsf{eff}}(t-t_0)}|\tilde{A}_i(t_0)\rangle = |\tilde{A}_i(t)\rangle \end{aligned}$$

We have effectively obtained a Q-hermitian Hamiltonian H_{eff} after a long time passed.

The normalized state $|A_i(t)\rangle_N \simeq |\tilde{A}_i(t)\rangle_N \equiv \frac{1}{\sqrt{\langle \tilde{A}_i(t)|_Q \ \tilde{A}_i(t) \rangle}} |\tilde{A}_i(t)\rangle$ and the expectation value of an operator O, $\langle \hat{O} \rangle_Q^{A_i A_i}(t) \simeq \langle \hat{O} \rangle_Q^{\tilde{A}_i \tilde{A}_i}(t) \equiv {}_N \langle \tilde{A}_i(t)|_Q O |\tilde{A}_i(t)\rangle_N$, obey

$$i\hbar \frac{\partial}{\partial t} |\tilde{A}_i(t)\rangle_N = \hat{H}_{\text{eff}} |\tilde{A}_i(t)\rangle_N,$$
 (2)

$$\frac{d}{dt}\langle \hat{O} \rangle_{Q}^{\tilde{A}_{i}\tilde{A}_{i}}(t) = -\frac{i}{\hbar} \langle \left[\hat{O}, \hat{H}_{\mathsf{eff}} \right] \rangle_{Q}^{\tilde{A}_{i}\tilde{A}_{i}}(t).$$
(3)

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

For a given ensemble $\{|A_i(t)\rangle\}$, let us consider a mixed state that is composed of $|A_i(t)\rangle_N$ with the probability q_i for each index i ($q_i \ge 0$, $\sum_i q_i = 1$).

We define the density matrix and expectation value of an operator \hat{O} for it by

$$\begin{split} \hat{\rho}_{Q}^{AA,\text{mixed}}(t) &\equiv \sum_{i} q_{i} |A_{i}(t)\rangle_{NN} \langle A_{i}(t)|_{Q} \equiv \sum_{i} q_{i} \hat{\rho}_{Q}^{A_{i}A_{i}}(t), \\ \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{AA,\text{mixed}}}(t) &\equiv \operatorname{tr} \left(\hat{\rho}_{Q}^{AA,\text{mixed}}(t) \hat{O} \right) \equiv \sum_{i} q_{i} \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{A_{i}A_{i}}}(t) = \sum_{i} q_{i} \langle \hat{O} \rangle_{Q}^{A_{i}A_{i}}(t), \end{split}$$

where
$$\hat{\rho}_Q^{A_iA_i}(t)$$
 obeys $\hat{\rho}_Q^{A_iA_i}(t)^2 = \hat{\rho}_Q^{A_iA_i}(t)$ and $\operatorname{tr}\left(\hat{\rho}_Q^{A_iA_i}(t)\right) = 1$. So $\operatorname{tr}\left(\hat{\rho}_Q^{AA,\operatorname{mixed}}(t)\right) = 1$.

They time-develop as follows:

$$\begin{aligned} & \frac{d}{dt} \hat{\rho}_{Q}^{AA,\text{mixed}}(t) \\ &= -\frac{i}{\hbar} \left[\hat{H}_{Qh}, \hat{\rho}_{Q}^{AA,\text{mixed}}(t) \right] - \frac{i}{\hbar} \sum_{i} q_{i} \left\{ \hat{\Delta} \left(\hat{H}_{Qa}; |A_{i}(t)\rangle_{N} \right), \hat{\rho}_{Q}^{A_{i}A_{i}} \right\}(t), \\ & \frac{d}{dt} \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{AA,\text{mixed}}}(t) \\ &= -\frac{i}{\hbar} \langle \left[\hat{O}, \hat{H}_{Qh} \right] \rangle_{\hat{\rho}_{Q}^{AA,\text{mixed}}}(t) - \frac{i}{\hbar} \sum_{i} q_{i} \langle \left\{ \hat{O}, \hat{\Delta} \left(\hat{H}_{Qa}; |A_{i}(t)\rangle_{N} \right) \right\} \rangle_{\hat{\rho}_{Q}^{A_{i}A_{i}}}(t). \end{aligned}$$

It is interesting that, in the classical limit, since $\langle \{\hat{O}, \hat{\Delta} (\hat{H}_{Qa}; |A_i(t)\rangle_N) \} \rangle_{\hat{\rho}_Q^{A_i A_i}}(t)$ is suppressed, Ehrenfest's theorem holds.

Now, let us consider the long time development. Then, since
$$|A_i(t)\rangle_N \simeq |\tilde{A}_i(t)\rangle_N$$
 obeys Eq.(2), we obtain the following relations for $\hat{\rho}_Q^{AA,\text{mixed}}(t) \simeq \hat{\rho}_Q^{\tilde{A}_i,\text{mixed}}(t), \hat{\rho}_Q^{A_iA_i}(t) \simeq \hat{\rho}_Q^{\tilde{A}_i,\tilde{A}_i}(t),$
 $\langle \hat{O} \rangle_{\hat{\rho}_Q^{AA,\text{mixed}}}(t) \simeq \langle \hat{O} \rangle_{\hat{\rho}_Q^{\tilde{A}},\tilde{A},\text{mixed}}(t), \text{ and } \langle \hat{O} \rangle_{\hat{\rho}_Q^{A_iA_i}}(t) \simeq \langle \hat{O} \rangle_{\hat{\rho}_Q^{\tilde{A}_i,\tilde{A}_i}}(t):$
 $\hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}(t) \equiv \sum_i q_i \hat{\rho}_Q^{\tilde{A}_i,\tilde{A}_i}(t) = \hat{U}_{\text{eff}}(t - T_A) \hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}(T_A) \hat{U}_{\text{eff}}(t - T_A)^{\dagger Q},$
 $\langle \hat{O} \rangle_{\hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}}(t) \equiv \text{tr} \left(\hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}(t) \hat{O} \right) \equiv \sum_i q_i \langle \hat{O} \rangle_{\hat{\rho}_Q^{\tilde{A}_i,\tilde{A}_i}}(t) = \sum_i q_i \langle \hat{O} \rangle_{\hat{\rho}_Q^{\tilde{A},\tilde{A}_i}}(t),$
 $\frac{d}{dt} \hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}(t) = -\frac{i}{\hbar} \left[\hat{H}_{\text{eff}}, \hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}(t) \right],$
 $\frac{d}{dt} \langle \hat{O} \rangle_{\hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}}(t) = -\frac{i}{\hbar} \langle [\hat{O}, \hat{H}_{\text{eff}}] \rangle_{\hat{\rho}_Q^{\tilde{A}\bar{A},\text{mixed}}}(t),$
where $\hat{U}_{\text{eff}}(t - T_A) \equiv e^{-\frac{i}{\hbar} \hat{H}_{\text{eff}}(t - T_A)}$ is *Q*-unitary, $U_{\text{eff}}^{\dagger Q} = U_{\text{eff}}^{-1}.$

We find that $\hat{\rho}_Q^{\tilde{A}\tilde{A},\text{mixed}}(t)$ obeys the von Neumann eq. with the *Q*-Hermitian Hamiltonian \hat{H}_{eff} and Ehrenfest's theorem holds. \Rightarrow the automatic hermiticity mechanism works for mixed states as well as for pure states in the future-not-included CAT. We introduce density matrices to describe mixed states in the future-included CAT, and 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 eq. $i\hbar \frac{d}{dt} |A_i(t)\rangle = \hat{H} |A_i(t)\rangle$ but also by $|B_i(t)\rangle$ that time-develops backward from the final time T_B according to $i\hbar \frac{d}{dt} |B_i(t)\rangle = \hat{H}^{\dagger Q} |B_i(t)\rangle \Leftrightarrow -i\hbar \frac{d}{dt} \langle B_i(t)|_Q = \langle B_i(t)|_Q \hat{H}.$

The states $|A_i(t)\rangle$ and $|B_i(t)\rangle$ are normalized by $\langle A_i(T_A)|_Q A_i(T_A)\rangle = \langle B_i(T_B)|_Q B_i(T_B)\rangle = 1.$

The normalized matrix element

$$\langle \hat{O} \rangle_{Q}^{B_{i}A_{i}}(t) \equiv \frac{\langle B_{i}(t)|_{Q}\hat{O}|A_{i}(t)\rangle}{\langle B_{i}(t)|_{Q}A_{i}(t)\rangle}$$
(4)

is a good candidate for an expectation value of an operator *O* in the future-included CAT, because, if it is viewed as such, we can obtain the Heisenberg eq., Ehrenfest's theorem, and a conserved probability current density.

Let us consider the other ensemble $\{|B_i(t)\rangle\}$ besides the ensemble $\{|A_i(t)\rangle\}$.

What kind of mixed states can be considered in the future-included theory?

One possible candidate:

the same type of mixed states as we considered above, which is described by the density matrix $\hat{\rho}_Q^{AA,\text{mixed}}(t)$ for $|A_i(t)\rangle$ and similar ones for $|B_i(t)\rangle$.

Introducing a normalized state and an expectation value of an operator O for it by $|B_i(t)\rangle_N \equiv \frac{1}{\sqrt{\langle B_i(t)|_Q B_i(t)\rangle}} |B_i(t)\rangle$ and $\langle \hat{O} \rangle_Q^{B_i B_i}(t) \equiv {}_N \langle B_i(t)|_Q O |B_i(t)\rangle_N$, which time-develop as $i\hbar \frac{\partial}{\partial t} |B_i(t)\rangle_N = \hat{H}_{Qh} |B_i(t)\rangle_N - \hat{\Delta} \left(\hat{H}_{Qa}; |B_i(t)\rangle_N\right) |B_i(t)\rangle_N$, $\frac{d}{dt} \langle \hat{O} \rangle_Q^{B_i B_i}(t) = -\frac{i}{\hbar} \langle \left[\hat{O}, \hat{H}_{Qh} \right] \rangle_Q^{B_i B_i}(t) + \frac{i}{\hbar} \langle \left\{ \hat{O}, \hat{\Delta} \left(\hat{H}_{Qa}; |B_i(t)\rangle_N \right) \right\} \rangle_Q^{B_i B_i}(t)$, we consider a mixed state that is given by $|B_i(t)\rangle_N$ with the probability r_i for each index i ($r_i \ge 0$, $\sum_i r_i = 1$).

We define the density matrix to describe the mixed state and the expectation value of *O* for it by

$$\begin{split} \hat{\rho}_{Q}^{BB,\text{mixed}}(t) &\equiv \sum_{i} r_{i} |B_{i}(t)\rangle_{NN} \langle B_{i}(t)|_{Q} \equiv \sum_{i} r_{i} \hat{\rho}_{Q}^{B_{i}B_{i}}(t), \\ \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{BB,\text{mixed}}}(t) &\equiv \operatorname{tr} \left(\hat{\rho}_{Q}^{BB,\text{mixed}}(t) \hat{O} \right) \equiv \sum_{i} r_{i} \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{B_{i}B_{i}}}(t) = \sum_{i} r_{i} \langle \hat{O} \rangle_{Q}^{B_{i}B_{i}}(t), \\ \text{where } \hat{\rho}_{Q}^{B_{i}B_{i}}(t) \text{ obeys } \hat{\rho}_{Q}^{B_{i}B_{i}}(t)^{2} = \hat{\rho}_{Q}^{B_{i}B_{i}}(t) \text{ and } \operatorname{tr} \left(\hat{\rho}_{Q}^{B_{i}B_{i}}(t) \right) = 1, \text{ so} \\ \operatorname{tr} \left(\hat{\rho}_{Q}^{BB,\text{mixed}}(t) \right) = 1. \end{split}$$

* $\hat{\rho}_Q^{BB,\text{mixed}}(t)$ and $\langle \hat{O} \rangle_{\hat{\rho}_Q^{BB,\text{mixed}}}(t)$ are *Q*-Hermitian and real for *Q*-Hermitian \hat{O} , respectively.

They time-develop as follows:

$$\begin{aligned} & \frac{d}{dt} \hat{\rho}_{Q}^{BB,\text{mixed}}(t) \\ &= -\frac{i}{\hbar} \left[\hat{H}_{Qh}, \hat{\rho}_{Q}^{BB,\text{mixed}}(t) \right] + \frac{i}{\hbar} \sum_{i} r_{i} \left\{ \hat{\Delta} \left(\hat{H}_{Qa}; |B_{i}(t)\rangle_{N} \right), \hat{\rho}_{Q}^{B_{i}B_{i}} \right\}(t), \\ & \frac{d}{dt} \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{BB,\text{mixed}}}(t) \\ &= -\frac{i}{\hbar} \langle \left[\hat{O}, \hat{H}_{Qh} \right] \rangle_{\hat{\rho}_{Q}^{BB,\text{mixed}}}(t) + \frac{i}{\hbar} \sum_{i} r_{i} \langle \left\{ \hat{O}, \hat{\Delta} \left(\hat{H}_{Qa}; |B_{i}(t)\rangle_{N} \right) \right\} \rangle_{\hat{\rho}_{Q}^{B_{i}B_{i}}}(t), \end{aligned}$$

which are almost the same as those for $\hat{\rho}_Q^{AA,\text{mixed}}(t)$. The only difference is that the sign in front of \hat{H}_{Qa} is opposite.

Using the automatic hermiticity mechanism: $|B_{i}(t)\rangle \simeq e^{\frac{1}{\hbar}B(T_{B}-t)}e^{-\frac{i}{\hbar}\hat{H}_{\text{eff}}(t-T_{B})}|\tilde{B}_{i}(T_{B})\rangle = \sum_{j\in A} b_{j}^{(i)}(t)|\lambda_{j}\rangle \equiv |\tilde{B}_{i}(t)\rangle,$ $|B_{i}(t)\rangle_{N} \simeq \frac{1}{\sqrt{\langle \tilde{B}_{i}(t)|_{Q} \ \tilde{B}_{i}(t)\rangle}}|\tilde{B}_{i}(t)\rangle \equiv |\tilde{B}_{i}(t)\rangle_{N} \text{ for large } T_{B} - t, \text{ we find that}$ the various relations for $\hat{\rho}_{Q}^{BB,\text{mixed}}(t) \simeq \hat{\rho}_{Q}^{\tilde{B}\tilde{B},\text{mixed}}(t)$ become the same as those for $\hat{\rho}_{Q}^{\tilde{A}\tilde{A},\text{mixed}}(t)$. $\label{eq:product} \begin{array}{l} \Rightarrow \mbox{The automatic hermiticity mechanism works for mixed states} \\ \mbox{described by the density matrices } \hat{\rho}_Q^{AA, {\rm mixed}}(t) \simeq \hat{\rho}_Q^{\tilde{A}\tilde{A}, {\rm mixed}}(t) \mbox{ and } \\ \hat{\rho}_Q^{BB, {\rm mixed}}(t) \simeq \hat{\rho}_Q^{\tilde{B}\tilde{B}, {\rm mixed}}(t). \end{array}$

- Via the mechanism, both of the density matrices nicely obey the von Neumann equation with the effectively obtained Q-Hermitian Hamiltonian \hat{H}_{eff} .
- $\hat{\rho}_Q^{A_iA_i}(t)$ and $\hat{\rho}_Q^{B_iB_i}(t)$ have real meanings as density matrices of $|A_i(t)\rangle_N$ and $|B_i(t)\rangle_N$.
- However, neither tr $(\hat{\rho}_Q^{A_iA_i}(t)\hat{O}) = {}_N\langle A_i(t)|_Q\hat{O}|A_i(t)\rangle_N$ nor tr $(\hat{\rho}_Q^{B_iB_i}(t)\hat{O}) = {}_N\langle B_i(t)|_Q\hat{O}|B_i(t)\rangle_N$ matches the normalized matrix element $\langle \hat{O} \rangle_Q^{B_iA_i}(t)$ given in Eq.(4).

In the future-included CAT, we have a philosophy s.t. it is not ${}_{N}\langle A_{i}(t)|_{Q}\hat{O}|A_{i}(t)\rangle_{N}$ nor ${}_{N}\langle B_{i}(t)|_{Q}\hat{O}|B_{i}(t)\rangle_{N}$ but $\langle \hat{O}\rangle_{Q}^{B_{i}A_{i}}(t)$ that has a role of an expectation value of \hat{O} .

 $\Rightarrow \hat{\rho}_Q^{A_i A_i}(t)$ and $\hat{\rho}_Q^{B_i B_i}(t)$ are not good in this sense.

 \Rightarrow Then, what should we adopt as a density matrix in the future-included CAT if we wish to respect the philosophy?

⇒ Let us consider the other kind of density matrix s.t. the trace of the product of each component with an index *i* and \hat{O} corresponds to $\langle \hat{O} \rangle_Q^{B_i A_i}(t)$.

Introducing $|A_i(t)\rangle_M \equiv \frac{|A_i(t)\rangle}{\sqrt{\langle B_i(t)|_Q A_i(t)\rangle}}$ and $|B_i(t)\rangle_M \equiv \frac{|B_i(t)\rangle}{\sqrt{\langle A_i(t)|_Q B_i(t)\rangle}}$, which obey $i\hbar \frac{d}{dt} |A_i(t)\rangle_M = \hat{H} |A_i(t)\rangle_M$, $i\hbar \frac{d}{dt} |B_i(t)\rangle_M = \hat{H}^{\dagger Q} |B_i(t)\rangle_M$, and $_M \langle B_i(t)|_Q A_i(t)\rangle_M = 1$, we define the "skew density matrix" $\hat{\rho}_Q^{BA,\text{mixed}}(t)$ and "expectation value" of \hat{O} for it by

$$\hat{\rho}_{Q}^{BA,\text{mixed}}(t) \equiv \sum_{i} s_{i} |A_{i}(t)\rangle_{MM} \langle B_{i}(t)|_{Q} \equiv \sum_{i} s_{i} \hat{\rho}_{Q}^{B_{i}A_{i}}(t),$$

$$\langle \hat{O} \rangle_{\hat{\rho}_{Q}^{BA,\text{mixed}}}(t) \equiv \operatorname{tr} \left(\hat{\rho}_{Q}^{BA,\text{mixed}}(t) \hat{O} \right) \equiv \sum_{i} s_{i} \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{B_{i}A_{i}}}(t) = \sum_{i} s_{i} \langle \hat{O} \rangle_{Q}^{B_{i}A_{i}}(t),$$

where the weight s_i for each $\hat{\rho}_Q^{B_iA_i}(t)$ obeys $s_i \ge 0$, $\sum_i s_i = 1$, and $\operatorname{tr}\left(\hat{\rho}_Q^{B_iA_i}(t)\right) = 1$, $\left(\hat{\rho}_Q^{B_iA_i}(t)\right)^2 = \hat{\rho}_Q^{B_iA_i}(t)$. So $\operatorname{tr}\left(\hat{\rho}_Q^{BA,\operatorname{mixed}}(t)\right) = 1$. $\hat{\rho}_Q^{BA,\operatorname{mixed}}(t) = \hat{U}(t-t_r)\hat{\rho}_Q^{BA,\operatorname{mixed}}(t_r)\hat{U}(t-t_r)^{-1}$, where $\hat{U}(t-t_r) \equiv e^{-\frac{i}{\hbar}\hat{H}(t-t_r)}$ is neither unitary nor Q-unitary, and t_r is a reference time. They time-develop as follows:

$$\begin{split} &\frac{d}{dt}\hat{\rho}_{Q}^{BA,\text{mixed}}(t) = -\frac{i}{\hbar}\left[\hat{H},\hat{\rho}_{Q}^{BA,\text{mixed}}(t)\right],\\ &\frac{d}{dt}\langle\hat{O}\rangle_{\hat{\rho}_{Q}^{BA,\text{mixed}}}(t) = -\frac{i}{\hbar}\langle\left[\hat{O},\hat{H}\right]\rangle_{\hat{\rho}_{Q}^{BA,\text{mixed}}}(t). \end{split}$$

 $\Rightarrow \hat{\rho}_Q^{BA,{\rm mixed}}(t)$ obeys the von Neumann eq. and Ehrenfest's theorem holds as they are.

These properties are quite in contrast to those of $\hat{\rho}_Q^{AA,\text{mixed}}(t)$ and $\hat{\rho}_Q^{BB,\text{mixed}}(t)$

If we consider the long time development, for

$$\begin{split} |A_{i}(t)\rangle_{M} &\simeq |\tilde{A}_{i}(t)\rangle_{M} \equiv \frac{|\tilde{A}_{i}(t)\rangle}{\sqrt{\langle \tilde{B}_{i}(t)|_{Q}\tilde{A}_{i}(t)\rangle}} \text{ and } \\ |B_{i}(t)\rangle_{M} &\simeq |\tilde{B}_{i}(t)\rangle_{M} \equiv \frac{|\tilde{B}_{i}(t)\rangle}{\sqrt{\langle \tilde{A}_{i}(t)|_{Q}\tilde{B}_{i}(t)\rangle}}, \\ \text{we find that} \\ \hat{\rho}_{Q}^{BA,\text{mixed}}(t) &\simeq \hat{\rho}_{Q}^{\tilde{B}\tilde{A},\text{mixed}}(t) \equiv \sum_{i} s_{i}|\tilde{A}_{i}(t)\rangle_{MM} \langle \tilde{B}_{i}(t)|_{Q} \equiv \sum_{i} s_{i}\hat{\rho}_{Q}^{\tilde{B}_{i}\tilde{A}_{i}}(t) \text{ and } \end{split}$$

$$\begin{split} & \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{B,\text{mixed}}}(t) \simeq \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{\tilde{B},\tilde{A},\text{mixed}}}(t) \equiv \text{tr} \left(\hat{\rho}_{Q}^{\tilde{B},\tilde{A},\text{mixed}}(t) \hat{O} \right) \\ & \equiv \sum_{i} s_{i} \langle \hat{O} \rangle_{\hat{\rho}_{Q}^{\tilde{B},\tilde{A}_{i}}}(t) = \sum_{i} s_{i} \langle \hat{O} \rangle_{Q}^{\tilde{B}_{i}\tilde{A}_{i}}(t) \text{ time-develop with an effectively} \end{split}$$

obtained Q-Hermitian Hamiltonian \hat{H}_{eff} as follows:

$$\begin{split} &\frac{d}{dt}\hat{\rho}_{Q}^{\tilde{B}\tilde{A},\text{mixed}}(t) = -\frac{i}{\hbar}\left[\hat{H}_{\text{eff}},\hat{\rho}_{Q}^{\tilde{B}\tilde{A},\text{mixed}}(t)\right],\\ &\frac{d}{dt}\langle\hat{O}\rangle_{\hat{\rho}_{Q}^{\tilde{B}\tilde{A},\text{mixed}}}(t) = -\frac{i}{\hbar}\langle\left[\hat{O},\hat{H}_{\text{eff}}\right]\rangle_{\hat{\rho}_{Q}^{\tilde{B}\tilde{A},\text{mixed}}}(t). \end{split}$$

However, $\hat{\rho}_{Q}^{\tilde{B}\tilde{A},\text{mixed}}(t)$, $\langle \hat{O} \rangle_{\hat{\rho}_{Q}^{\tilde{B}\tilde{A},\text{mixed}}(t)}$ 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 $\hat{\rho}_Q^{AA,\text{mixed}}(t)$ and $\hat{\rho}_Q^{BB,\text{mixed}}(t)$, where only either $|A_i(t)\rangle_N$ or $|B_i(t)\rangle_N$ is used.

 \Rightarrow To resolve this problem, we will consider it in another way.

On the skew density matrix

$$\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA,\text{mixed}}}(t) = \sum_i s_i \operatorname{tr} \left(\hat{\rho}_Q^{B_i A_i}(t) \hat{O} \right) = \sum_i s_i \frac{\operatorname{tr} \left(\hat{\rho}_Q^{B_i B_i}(t) \hat{O}_Q^{A_i A_i}(t) \right)}{\operatorname{tr} \left(\hat{\rho}_Q^{B_i B_i}(t) \hat{\rho}_Q^{A_i A_i}(t) \right)} \text{ for } Q = 1$$

corresponds to the weak value for the generalized state (Y. Aharonov ,L. Vaidman, 1991), but is different from the generalized weak value $\frac{\text{tr}(\hat{\rho}_f \hat{O} \hat{\rho}_i)}{\text{tr}(\hat{\rho}_f \hat{\rho}_i)}$ (S. Wu, K. Mølmer, 2009, S. Tamate, T. Nakanishi, and M. Kitano, 2012).

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. Then, in a situation s.t. a pair $\{|A_i\rangle, |B_i\rangle\}$ and each weight $\{s_i\}$ are given, our skew density matrix enables us to calculate and simulate the "expectation value" of *O*. Hermiticity and reality for $\hat{\rho}_Q^{BA,\text{mixed}}(t)$ and $\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA,\text{mixed}}}(t)$

KN and H. B. Nielsen, PTEP **2013**, 023B04; **2018**, 039201[erratum].

We previously obtained the correspondence:

$$\langle O \rangle^{BA}$$
 for large $T_B - t$ and large $t - T_A \simeq \langle O \rangle^{AA}_{Q'}$ for large $t - T_A$,

based on the Schrödinger eq.(1) and $i\hbar \frac{d}{dt}|B(t)\rangle = H^{\dagger}|B(t)\rangle$, where $\langle O \rangle^{BA} = \frac{\langle B(t)|O|A(t)\rangle}{\langle B(t)|A(t)\rangle}$ and $\langle O \rangle^{AA}_{Q'} = \frac{\langle A(t)|_{Q'}O|A(t)\rangle}{\langle A(t)|_{Q'}A(t)\rangle}$.

 \Rightarrow The future-included CAT is not excluded phenomenologically, even though it looks very exotic.

We estimate $\langle O \rangle_Q^{BA}$ and $\hat{\rho}_Q^{BA}(t)$, based on the Schrödinger eq.(1) and $i\hbar \frac{d}{dt} |B(t)\rangle = H^{\dagger^Q} |B(t)\rangle$.

We express
$$\langle O \rangle_Q^{BA}$$
 as $\langle O \rangle_Q^{BA}(t) = \frac{\langle A(t)|_Q B(t) \rangle \langle B(t)|_Q O|A(t) \rangle}{\langle A(t)|_Q B(t) \rangle \langle B(t)|_Q A(t) \rangle}$.

Utilizing the expansion: $|B(T_B)\rangle = \sum_i c_i |\lambda_i\rangle = \sum_i J(\lambda_i)^* |\lambda_i\rangle$, where $J(\lambda_i)$ is a function of λ_i , we evaluate $|B(t)\rangle\langle B(t)|_Q$ as follows:

$$\begin{split} |B(t)\rangle\langle B(t)|_{Q} &= e^{-\frac{i}{\hbar}\hat{H}^{\dagger Q}(t-T_{B})}|B(T_{B})\rangle\langle B(T_{B})|_{Q}e^{\frac{i}{\hbar}\hat{H}(t-T_{B})} \\ &= \sum_{i,j}c_{i}c_{j}^{*}e^{\frac{i}{\hbar}\mathsf{Re}(\lambda_{j}-\lambda_{i})(t-T_{B})}e^{\frac{1}{\hbar}\mathsf{Im}(\lambda_{j}+\lambda_{i})(T_{B}-t)}|\lambda_{i}\rangle\langle\lambda_{j}|_{Q} \\ &\simeq \frac{\int_{t-\Delta t}^{t+\Delta t}|B(t)\rangle\langle B(t)|_{Q}dt}{\int_{t-\Delta t}^{t+\Delta t}dt} \simeq \sum_{i}|c_{i}|^{2}e^{\frac{2}{\hbar}\mathsf{Im}\lambda_{i}(T_{B}-t)}|\lambda_{i}\rangle\langle\lambda_{i}|_{Q} \\ &\simeq e^{\frac{2}{\hbar}B(T_{B}-t)}Q_{4} \quad \text{for large } T_{B}-t, \end{split}$$

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 $Q_4 \equiv \sum_{i \in A} |c_i|^2 |\lambda_i\rangle \langle \lambda_i|_Q = J(\hat{H}_{eff} + iB\Lambda_A)^{\dagger Q} \Lambda_A J(\hat{H}_{eff} + iB\Lambda_A) = Q^{-1} \tilde{J}(\hat{H}_{eff})^{\dagger} Q \tilde{J}(\hat{H}_{eff}) \equiv Q^{-1} Q_{\tilde{J}}.$

Here, supposing that $\operatorname{Re}\lambda_i$ are not degenerate, we have introduced $\Lambda_A \equiv \sum_{i \in A} |\lambda_i\rangle \langle \lambda_i|_Q$, a function \tilde{J} s.t. $\tilde{J}(\operatorname{Re}\lambda_i) \equiv J(\operatorname{Re}\lambda_i + iB) = c_i^*$ for $i \in A$, and $Q_{\tilde{J}} \equiv \tilde{J}(\hat{H}_{eff})^{\dagger}Q\tilde{J}(\hat{H}_{eff})$.

Now we use the automatic hermiticity mechanism for large $t - T_A$. Then, since $|A(t)\rangle \equiv \sum_i a_i(t) |\lambda_i\rangle$ behaves as $|\tilde{A}(t)\rangle \equiv \sum_{i \in A} a_i(t) |\lambda_i\rangle$, we obtain

$$\langle O \rangle_{Q}^{BA} \simeq \frac{\langle \tilde{A}(t)|_{Q_{\tilde{J}}} O | \tilde{A}(t) \rangle}{\langle \tilde{A}(t)|_{Q_{\tilde{J}}} \tilde{A}(t) \rangle} \equiv \langle O \rangle_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A}} \quad \text{for large } T_{B} - t \text{ and large } t - T_{A}.$$
(6)

Next, let us consider the expectation value in the future-not-included theory: $\langle O \rangle_{Q_J}^{AA} \equiv \frac{\langle A(t)|_{Q_J}O|A(t) \rangle}{\langle A(t)|_{Q_J}A(t) \rangle}$, where $Q_J \equiv J(\hat{H})^{\dagger}QJ(\hat{H}) = (P_{J^{-1}}^{-1})^{\dagger}P_{J^{-1}}^{-1}$, 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 $|\lambda_i\rangle^{J^{-1}} \equiv J(\hat{H})^{-1}|\lambda_i\rangle$, so that $|\lambda_i\rangle^{J^{-1}}$ is Q_J -orthogonal, i.e., $I_{Q_J}(|\lambda_i\rangle^{J^{-1}}, |\lambda_j\rangle^{J^{-1}}) \equiv {}^{J^{-1}}\langle\lambda_i|Q_J|\lambda_j\rangle^{J^{-1}} = \delta_{ij}$. We use the automatic hermiticity mechanism for large $t - T_A$. $|A(t)\rangle$ behaves as $|\tilde{A}(t)\rangle = \sum_{i \in A} a_i(t)|\lambda_i\rangle$, and Q_J is estimated as follows:

$$Q_J \simeq J(\hat{H}_{\mathsf{eff}} + iB\Lambda_A)^{\dagger}QJ(\hat{H}_{\mathsf{eff}} + iB\Lambda_A) = \tilde{J}(\hat{H}_{\mathsf{eff}})^{\dagger}Q\tilde{J}(\hat{H}_{\mathsf{eff}}) = Q_{\tilde{J}}.$$

Then we find
$$\langle O \rangle_{Q_J}^{AA} \simeq \frac{\langle \tilde{A}(t) | Q_{\tilde{J}} O | \tilde{A}(t) \rangle}{\langle \tilde{A}(t) | Q_{\tilde{J}} \tilde{A}(t) \rangle} = \langle O \rangle_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A}}$$
 for large $t - T_A$.

Thus we have obtained the following correspondence:

$$\langle O \rangle_Q^{BA}$$
 for large $T_B - t$ and large $t - T_A \simeq \langle O \rangle_{Q_J}^{\tilde{A}\tilde{A}}$
 $\simeq \langle O \rangle_{Q_J}^{AA}$ for large $t - T_A$,

which suggests that the future-included theory is not excluded, although it looks very exotic.

 $\langle O \rangle_{Q_{j}}^{\tilde{A}\tilde{A}}$ is real for Q_{j} -Hermitian O, and time-develops according to the Q_{j} -Hermitian Hamiltonian \hat{H}_{eff} .

We can apply this correspondence to each *i*-component $\langle \hat{O} \rangle_{O}^{B_{i}A_{i}}(t)$.

Next let us evaluate the skew density matrix $\hat{\rho}_Q^{BA}(t) = \frac{|A(t)\rangle\langle B(t)|_Q}{\langle B(t)|_Q A(t)\rangle}$ by multiplying it by $1 = \frac{\langle A(t)|_Q B(t)\rangle}{\langle A(t)|_Q B(t)\rangle}$. Utilizing the above evaluation of $|B(t)\rangle\langle B(t)|_Q$, we obtain the correspondence:

$$\hat{\rho}_Q^{BA}(t)$$
 for large $T_B - t$ and large $t - T_A \simeq \hat{\rho}_{Q_J}^{\tilde{A}\tilde{A}}(t)$
 $\simeq \hat{\rho}_{Q_J}^{AA}(t)$ for large $t - T_A$,

where
$$\hat{\rho}_{Q_{J}}^{\tilde{A}\tilde{A}}(t) \equiv \frac{|\tilde{A}(t)\rangle\langle\tilde{A}(t)|_{Q_{J}}}{\langle\tilde{A}(t)|_{Q_{J}}\tilde{A}(t)\rangle} = \hat{U}_{\text{eff}}(t-t_{r})\hat{\rho}_{Q_{J}}^{\tilde{A}\tilde{A}}(t_{r})\hat{U}_{\text{eff}}(t-t_{r})^{\dagger^{Q_{J}}}.$$

Here t_r is a reference time, and $\hat{\rho}_{Q_J}^{\tilde{A}\tilde{A}}(t)$ obeys $\operatorname{tr}\left(\hat{\rho}_{Q_J}^{\tilde{A}\tilde{A}}\right) = 1$ and $\left(\hat{\rho}_{Q_J}^{\tilde{A}\tilde{A}}\right)^2 = \hat{\rho}_{Q_J}^{\tilde{A}\tilde{A}}$.

 $\hat{U}_{\text{eff}}(t-t_r) = e^{-\frac{i}{\hbar}\hat{H}_{\text{eff}}(t-t_r)}$ is $Q_{\tilde{J}}$ -unitary, and $\hat{\rho}_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A}}(t)$ is $Q_{\tilde{J}}$ -Hermitian.

We can apply this correspondence to each *i*-component $\hat{\rho}_Q^{B_i A_i}(t)$.

Therefore, though our skew density matrix $\hat{\rho}_Q^{B_iA_i}(t)$ is not Q-Hermitian by its definition, after a long time development it results in a usual expression of density matrix $\hat{\rho}_{Q_j}^{\tilde{A}_i\tilde{A}_i}(t)$ that is $Q_{\tilde{J}}$ -Hermitian.

Application to $\hat{\rho}_Q^{BA,\text{mixed}}(t) = \sum_i s_i \hat{\rho}_Q^{B_i A_i}(t)$ is rather straightforward and we easily see that it time-develops similarly.

Indeed, applying this correspondence to each component $\hat{\rho}_Q^{B_iA_i}(t)$, we find that the expectation value of O for $\hat{\rho}_Q^{B_iA_i}(t)$, $\langle \hat{O} \rangle_{\hat{\rho}_Q^{B_iA_i}}(t)$, is expressed for large $T_B - t$ and large $t - T_A$ as

$$\langle \hat{O} \rangle_{\hat{\rho}_{Q}^{B_{i}A_{i}}}(t) = \operatorname{tr}\left(\hat{\rho}_{Q}^{B_{i}A_{i}}(t)\hat{O}\right) \simeq \operatorname{tr}\left(\hat{\rho}_{Q_{J}}^{\tilde{A}_{i}\tilde{A}_{i}}(t)\hat{O}\right) \equiv \langle \hat{O} \rangle_{\hat{\rho}_{Q_{J}}^{\tilde{A}_{i}\tilde{A}_{i}}}(t) = \langle O \rangle_{Q_{J}}^{\tilde{A}_{i}\tilde{A}_{i}}(t),$$

which is real for $Q_{\tilde{J}}$ -Hermitian O.

Finally, $\hat{\rho}_{Q}^{BA,\text{mixed}}(t) \simeq \hat{\rho}_{Q_{J}}^{\tilde{A}\tilde{A},\text{mixed}}(t) = \sum_{i} s_{i} \hat{\rho}_{Q_{J}}^{\tilde{A}_{i}\tilde{A}_{i}}(t)$ and $\langle \hat{O} \rangle_{\hat{\rho}_{Q}^{BA,\text{mixed}}}(t) \simeq \langle \hat{O} \rangle_{\hat{\rho}_{Q_{J}}^{\tilde{A}\tilde{A},\text{mixed}}}(t) = \sum_{i} s_{i} \langle \hat{O} \rangle_{\hat{\rho}_{Q_{J}}^{\tilde{A}_{i}\tilde{A}_{i}}}(t)$ time-develop according to

$$\frac{d}{dt}\hat{\rho}_{Q_{J}}^{\tilde{A}\tilde{A},\text{mixed}}(t) = -\frac{i}{\hbar} \Big[\hat{H}_{\text{eff}}, \hat{\rho}_{Q_{J}}^{\tilde{A}\tilde{A},\text{mixed}}(t) \Big], \tag{7}$$

$$\frac{d}{dt}\langle \hat{O} \rangle_{\hat{\rho}_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A},\text{mixed}}}(t) = -\frac{i}{\hbar} \langle \left[\hat{O}, \hat{H}_{\text{eff}} \right] \rangle_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A},\text{mixed}}(t),$$
(8)

which show that $\hat{\rho}_Q^{BA,\text{mixed}}(t) \simeq \hat{\rho}_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A},\text{mixed}}(t)$ obeys the von Neumann equation with the $Q_{\tilde{J}}$ -Hermitian Hamiltonian \hat{H}_{eff} and Ehrenfest's theorem holds.

* $\hat{\rho}_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A},\text{mixed}}(t)$ is $Q_{\tilde{J}}$ -Hermitian, and $\langle \hat{O} \rangle_{\hat{\rho}_{Q_{\tilde{J}}}^{\tilde{A}\tilde{A},\text{mixed}}}(t)$ is real for $Q_{\tilde{J}}$ -Hermitian O.

⇒ The problem with $\hat{\rho}_Q^{BA,\text{mixed}}(t)$ and $\langle \hat{O} \rangle_{\hat{\rho}_Q^{BA,\text{mixed}}}(t)$ mentioned above has been effectively resolved by considering the long time development for large $T_B - t$ and large $t - T_A$.

Summary and outlook

We studied a couple of density matrices to deal with mixed states. In particular, we investigated the skew density matrix $\hat{\rho}_Q^{BA,\text{mixed}}(t)$ that has nice properties in the future-included CAT.

Utilizing the density matrices, it would be intriguing to study

- the von Neumann entropy
- classical dynamics via Wigner function
- master equation by interpreting our theory as a subsystem in a larger system
- provide $\langle \hat{O} \rangle_{\text{periodic time}}$ with the time *t* dependence by introducing a clock operator $\hat{T}_{\text{clock}}(t)$ in a periodic universe model that we previously studied

KN, H.B.Nielsen, PTEP 2022 091B01

• investigate the harmonic oscillator that we previously studied more in detail, and the extention of the *Q*-Hilbert space

KN, H.B.Nielsen, PTEP 2019 073B01

Complex coordinate and momentum formalism

KN and H.B.Nielsen, PTP126 (2011)1021

q and p easily get complex.

How is $\psi(q) = \langle q | \psi \rangle$ expressed for complex *q*?

We proposed for complex q and p

$$m\langle_{new} q | \hat{q}_{new} = m \langle_{new} q | q,$$

$$m\langle_{new} p | \hat{p}_{new} = m \langle_{new} p | p.$$

 $_m \langle_{new} q| \equiv \langle_{new} q^*|$: a modified bra defined to keep the analyticity in dynamical parameters such as q and p

We also introduced mathematical devices such as modified bras, modified complex conjugate, and a smeared delta function etc. for complex values, to keep the analyticity. \rightarrow we can express complex saddle points in terms of bras and kets.

Comparison between the future-included and future-not-included CAT

	Future-included CAT	Future-not-included
		CAT
action	$S = \int_{T_A}^{T_B} dt L$	$S = \int_{T_A}^t dt L$
"exp. value"	$\langle \hat{O} \rangle^{BA} = \frac{\langle B(t) \hat{O} A(t) \rangle}{\langle B(t) A(t) \rangle}$	$\langle \hat{O} \rangle^{AA} = \frac{\langle A(t) \hat{O} A(t) \rangle}{\langle A(t) A(t) \rangle}$
time	$i\hbar \frac{d}{dt} \langle \hat{O} \rangle^{BA}$	$i\hbar \frac{d}{dt} \langle \hat{O} \rangle^{AA}$
development	$=\langle [\hat{O}, \hat{H}] \rangle^{BA}$	$\simeq \langle [\hat{O}, \hat{H}_h] \rangle^{AA}$
classical theory	$\delta S = 0$	$\delta S_{\text{eff}} = 0,$
		$S_{\text{eff}} = \int_{T_A}^t dt L_{\text{eff}} \in \mathbf{R}$
momentum	$p = m\dot{q},$	$p = m_{\text{eff}} \dot{q},$
relation	$m = m_R + im_I \in \mathbf{C}$	$m_{\text{eff}} \equiv m_R + \frac{m_I^2}{m_R} \in \mathbf{R}$

K.N., H.B.Nielsen, IJMP **A27**(2012) 1250076;Erratum-ibid, **A32**(2017) 1792003 K.N., H.B.Nielsen, PTEP **2013** 023B04; Erratum-ibid, **2018** 039201 K.N., H.B.Nielsen, PTEP **2013** 073A03; Erratum-ibid, **2018** 029201

Complex action suggests future-included theory

KN and H.B.Nielsen, PTEP 2017 111B01

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 theory.

Otherwise, we encounter a contradiction: persons living at different times would be led to a strange re-choosing of initial states, and see different histories of the universe.

 \Rightarrow The future-not-included CAT is excluded.

Even so, the future-not-included CAT still remains to be fascinating: a good playground to study various intriguing aspects of the CAT.

Theorem on the normalized matrix element $\langle \hat{O} \rangle_{O}^{BA}$

KN, H.B.Nielsen, PTEP 2015 051B01; PTEP 2017 081B01

Theorem Assume that \hat{H} is non-normal but diagonalizable and that the imaginary part of its eigenvalues are bounded from above, and define a modified inner product I_Q . Let $|A(t)\rangle$ and $|B(t)\rangle$ time-develop according to $|A(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t-T_A)}|A(T_A)\rangle$, $|B(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}^{\dagger Q}(t-T_B)}|B(T_B)\rangle$, and be normalized by $\langle A(T_A)|_Q A(T_A)\rangle = 1$, $\langle B(T_B)|_Q B(T_B)\rangle = 1$. Next determine $|A(T_A)\rangle$ and $|B(T_B)\rangle$ so as to maximize $|\langle B(t)|_Q A(t)\rangle|$. Then, provided that $\hat{O}^{\dagger Q} = \hat{O}$, $\langle \hat{O} \rangle_Q^{BA} \equiv \frac{\langle B(t)|_Q \hat{O}|A(t)\rangle}{\langle B(t)|_Q A(t)\rangle}$ becomes real and time-develops under a *Q*-Hermitian Hamiltonian.

We call this way of thinking the maximization principle.

* Im λ_i are bounded from above to avoid the Feynman path integral $\int e^{\frac{i}{\hbar}S} \mathcal{D}$ path being divergently meaningless.

 \Rightarrow Some Im λ_i take the maximal value *B*, and we denote the corresponding subset of $\{i\}$ as *A*.

Among the four types of quantum theory, only in the future-included CAT, initial (and final) conditions are determined in the Feynman path integral. \leftarrow One of the benefits of the CAT.

Periodic complex action theory

KN, H.B.Nielsen, PTEP 2022 091B01

In the periodic CAT, extending the weak value of \hat{O} to

 $\langle \hat{O} \rangle_{\text{periodic time}} \equiv \frac{\text{Tr}\left(e^{-\frac{i}{\hbar}\hat{H}t_p}\hat{O}\right)}{\text{Tr}\left(e^{-\frac{i}{\hbar}\hat{H}t_p}\right)}$, we presented a theorem stating that $\langle \hat{O} \rangle_{\text{periodic time}}$ becomes real provided that \hat{O} is *Q*-Hermitian, for the period t_p selected s.t. $|\text{Tr}\left(e^{-\frac{i}{\hbar}\hat{H}t_p}\right)|$ is maximized, in the case where $B \leq 0$ and $|B| << |\text{Re}\lambda_m - \text{Re}\lambda_n|$ for $\forall m, n \ (m \neq n)$.

The theorem suggests that, if our universe is periodic, then even the period could be an adjustment parameter to be determined in the Feynman path integral.

This is a variant of the maximization principle that we previously proposed.