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*Published in:*  
Progress of Theoretical and Experimental Physics

*DOI:*  
[10.1093/ptep/ptv057](https://doi.org/10.1093/ptep/ptv057)

*Publication date:*  
2015

*Document version*  
Publisher's PDF, also known as Version of record

*Citation for published version (APA):*  
Nagao, K., & Nielsen, H. F. B. (2015). Reality and hermiticity from maximizing overlap in the future-included complex action theory. *Progress of Theoretical and Experimental Physics*, 2015(5), [051B01].  
<https://doi.org/10.1093/ptep/ptv057>

## Letter

**Reality and hermiticity from maximizing overlap in the future-included complex action theory**Keiichi Nagao<sup>1,\*</sup> and Holger Bech Nielsen<sup>2,\*</sup><sup>1</sup>*Faculty of Education, Ibaraki University, Mito 310-8512 Japan*<sup>2</sup>*Niels Bohr Institute, University of Copenhagen, 17 Blegdamsvej, Copenhagen  $\phi$ , Denmark*

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Received February 5, 2015; Revised March 11, 2015; Accepted March 24, 2015; Published May 11, 2015

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 In the complex action theory whose path runs over not only past but also future, we study a normalized matrix element of an operator  $\hat{O}$  defined in terms of the future state at the latest time  $T_B$  and the past state at the earliest time  $T_A$  with a proper inner product that makes normal a given Hamiltonian that is non-normal at first. We present a theorem that states that, provided that the operator  $\hat{O}$  is  $Q$ -Hermitian, i.e., Hermitian with regard to the proper inner product, the normalized matrix element 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 from the past state to the future state is maximized. Furthermore, we give a possible procedure to formulate the  $Q$ -Hermitian Hamiltonian in terms of  $Q$ -Hermitian coordinate and momentum operators, and construct a conserved probability current density.  
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Subject Index    A60, B30

1. *Introduction* The complex action theory (CAT) is a trial to extend quantum theories so that the action is complex at a fundamental level, but effectively looks real. So far, the CAT has been investigated with the expectation that the imaginary part of the action would give some falsifiable predictions [1–4], and various interesting suggestions have been made 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]. In the CAT, the Hamiltonian  $\hat{H}$  is generically non-normal, so it is not contained in the class of PT-symmetric non-Hermitian Hamiltonians that have been intensively studied [13–16]. In Ref. [17], introducing what we call the proper inner product  $I_Q$  so that the eigenstates of the Hamiltonian become orthogonal to each other with respect to it, we presented a mechanism to effectively obtain a Hamiltonian that is  $Q$ -Hermitian, i.e., Hermitian with respect to the proper inner product, after a long time development. In Ref. [18], we proposed a complex coordinate and momentum formalism by explicitly constructing non-Hermitian operators of complex coordinate  $q$  and momentum  $p$  and their eigenstates, so that we can deal with complex  $q$  and  $p$  properly. In general, the CAT could be classified into two theories: one is the future-not-included theory, i.e., the theory including only a past time as an integration interval of time, and the other one is the future-included theory [1], which includes not only a past time but also a future time. Using the complex coordinate and momentum formalism [18] in the Feynman path integral, we found that the momentum relation is given by the usual expression  $p = m\dot{q}$ , where  $m$  is a complex

mass, in the future-included theory [19], and another expression  $p = \left(m_R + \frac{m_I^2}{m_R}\right)\dot{q}$ , where  $m_R$  and  $m_I$  are the real and imaginary parts of  $m$ , respectively, in the future-not-included theory [20]. The future-included theory is described by using the future state  $|B(T_B)\rangle$  at the final time  $T_B$  and the past state  $|A(T_A)\rangle$  at the initial time  $T_A$ . In Refs. [21,22] we studied the normalized matrix element<sup>1</sup>  $\langle\hat{O}\rangle^{BA} \equiv \frac{\langle B(t)|\hat{O}|A(t)\rangle}{\langle B(t)|A(t)\rangle}$ , where  $t$  is an arbitrary time ( $T_A \leq t \leq T_B$ ), in the future-included theory, and found that, if we regard  $\langle\hat{O}\rangle^{BA}$  as an expectation value in the future-included theory, then we obtain the Heisenberg equation, Ehrenfest's theorem, and a conserved probability current density. This suggests that  $\langle\hat{O}\rangle^{BA}$  is a strong candidate for an expectation value in the future-included theory.

In this letter we study in the future-included CAT a slightly modified quantity  $\langle\hat{O}\rangle_Q^{BA} \equiv \frac{\langle B(t)|_Q\hat{O}|A(t)\rangle}{\langle B(t)|_QA(t)\rangle}$ , where  $\langle B(t)|_Q \equiv \langle B(t)|Q$ , and  $Q$  is a Hermitian operator<sup>2</sup> that is used to define the proper inner product  $I_Q$ . The choice of  $\langle\hat{O}\rangle_Q^{BA}$  or  $\langle\hat{O}\rangle^{BA}$  is only a matter of notation as to what the state symbol  $\langle B(t)|$  shall precisely mean. On the other hand, the choice of the inner product used in the normalization of the initial and final states  $|A(T_A)\rangle$  and  $\langle B(T_B)|$  is not just a matter of notation, once we have chosen  $\langle\hat{O}\rangle_Q^{BA}$  as the expression of the candidate for our expectation value. That is to say, according to the choice of the inner product used in the normalization of the initial and final states, two slightly different versions could be defined. The normalization defined with the usual inner product  $I$  has the true meaning of normalization, of course, but includes unphysical transitions between different eigenstates with different eigenvalues of the Hamiltonian  $\hat{H}$ . The normalization defined with the proper inner product  $I_Q$ , which we call  $Q$ -normalization, excludes such unphysical transitions, but does not have the original meaning of normalization. Thus, each choice seems to have both advantages and disadvantages, so we are interested in the study of both versions. However, let us admit that, in the version with the usually normalized initial and final states, it is not easy to evaluate  $\langle\hat{O}\rangle_Q^{BA}$  clearly, because we cannot exhaustively make use of the orthogonality of the eigenstates of the Hamiltonian  $\hat{H}$ . Therefore, we postpone the study of this version to the future, and concentrate in this letter on the analysis of the version with the  $Q$ -normalized initial and final states, which is much easier to study than the other version.

Assuming that a given Hamiltonian  $\hat{H}$  is non-normal but diagonalizable, and that the imaginary parts of the eigenvalues of  $\hat{H}$  are bounded from above, we present a theorem that claims that  $\langle\hat{O}\rangle_Q^{BA}$  becomes real and time-develops under a  $Q$ -Hermitian Hamiltonian for any  $Q$ -Hermitian operator  $\hat{O}$ , provided that  $|B(t)\rangle$  and  $|A(t)\rangle$  are the time-developed states maximizing the absolute value of the transition amplitude  $|\langle B(t)|_QA(t)\rangle|$ . Such states would represent an approximation to  $|\langle B(t)|_QA(t)\rangle|$  in the situation that  $|B(T_B)\rangle$  and  $|A(T_A)\rangle$  were randomly given. In fact, in the large  $T \equiv T_B - T_A$  case, only terms associated with the largest imaginary parts of the eigenvalues of the Hamiltonian would dominate, and even with random initial and final states the dominant term would give the biggest value. We call this thinking the maximization principle. We shall prove this theorem by finding that  $\langle\hat{O}\rangle_Q^{BA}$  for the states maximizing  $|\langle B(t)|_QA(t)\rangle|$  becomes an expression similar to an expectation value defined with  $I_Q$  in the future-not-included theory. Indeed, it is very important to obtain a real expectation value and a Hermitian Hamiltonian in the CAT so that it can survive as

<sup>1</sup> In the real action theory (RAT), the normalized matrix element  $\langle\hat{O}\rangle^{BA}$  is called the weak value [23], and has been intensively studied. For details, see Ref. [24] and references therein.

<sup>2</sup> In the special case of the Hamiltonian  $\hat{H}$  being Hermitian,  $Q$  is just a unit operator, so  $\langle\hat{O}\rangle_Q^{BA}$  corresponds to  $\langle\hat{O}\rangle^{BA}$ .

a possible true fundamental quantum theory. The maximization principle is regarded as a method of obtaining not only a real expectation value but also a  $Q$ -Hermitian Hamiltonian. Furthermore, assuming that the non-normal Hamiltonian given at first is written in terms of the Hermitian coordinate and momentum operators  $\hat{q}$  and  $\hat{p}$ , we give a possible procedure to formulate the  $Q$ -Hermitian Hamiltonian in terms of  $Q$ -Hermitian coordinate and momentum operators  $\hat{q}_Q$  and  $\hat{p}_Q$ . We also provide a  $Q$ -Hermitian probability density operator and construct a conserved probability current density.

**2. Proper inner product and future-included complex action theory** We consider a general non-normal diagonalizable Hamiltonian  $\hat{H}$ , i.e.,  $[\hat{H}, \hat{H}^\dagger] \neq 0$ , for a general quantum mechanical system that could be the whole world, and review a proper inner product for  $\hat{H}$  that makes  $\hat{H}$  normal with respect to it by following Refs. [17,18]. We define the eigenstates  $|\lambda_i\rangle (i = 1, 2, \dots)$  of  $\hat{H}$  such that

$$\hat{H}|\lambda_i\rangle = \lambda_i|\lambda_i\rangle, \quad (1)$$

where  $\lambda_i (i = 1, 2, \dots)$  are the eigenvalues of  $\hat{H}$ , and introduce the diagonalizing operator  $P = (|\lambda_1\rangle, |\lambda_2\rangle, \dots)$ , so that  $\hat{H}$  is diagonalized as  $\hat{H} = PDP^{-1}$ , where  $D$  is given by  $\text{diag}(\lambda_1, \lambda_2, \dots)$ . Let us consider a transition from an eigenstate  $|\lambda_i\rangle$  to another  $|\lambda_j\rangle$  ( $i \neq j$ ) fast in time  $\Delta t$ . Since  $|\lambda_i\rangle$  are not orthogonal to each other in the usual inner product  $I$ ,  $I(|\lambda_i\rangle, |\lambda_j\rangle) \equiv \langle \lambda_i | \lambda_j \rangle \neq \delta_{ij}$ , the transition can be measured, i.e.,  $|I(|\lambda_j\rangle, \exp(-\frac{i}{\hbar}\hat{H}\Delta t)|\lambda_i\rangle)|^2 \neq 0$ , though  $\hat{H}$  cannot bring the system from  $|\lambda_i\rangle$  to  $|\lambda_j\rangle$  ( $i \neq j$ ). Such an unphysical transition from one eigenstate to another with a different eigenvalue should be prohibited in a reasonable theory. In order to have reasonable probabilistic results, we introduce a proper inner product [17,18]<sup>3</sup> for arbitrary kets  $|u\rangle$  and  $|v\rangle$  as

$$I_Q(|u\rangle, |v\rangle) \equiv \langle u|_Q v \rangle \equiv \langle u|Q|v\rangle, \quad (2)$$

where  $Q$  is a Hermitian operator chosen as  $Q = (P^\dagger)^{-1}P^{-1}$ , so that  $|\lambda_i\rangle$  become orthogonal to each other with regard to  $I_Q$ :

$$\langle \lambda_i |_Q \lambda_j \rangle = \delta_{ij}. \quad (3)$$

This implies the orthogonality relation  $\sum_i |\lambda_i\rangle \langle \lambda_i|_Q = 1$ . In the special case of the Hamiltonian  $\hat{H}$  being Hermitian,  $Q$  would be the unit operator. We introduce the “ $Q$ -Hermitian” conjugate  $\dagger^Q$  of an operator  $A$  by  $\langle \psi_2 |_Q A | \psi_1 \rangle^* \equiv \langle \psi_1 |_Q A^{\dagger^Q} | \psi_2 \rangle$ , so

$$A^{\dagger^Q} \equiv Q^{-1} A^\dagger Q. \quad (4)$$

If  $A$  obeys  $A^{\dagger^Q} = A$ ,  $A$  is  $Q$ -Hermitian. We also define  $\dagger^Q$  for kets and bras as  $|\lambda\rangle^{\dagger^Q} \equiv \langle \lambda |_Q$  and  $(\langle \lambda |_Q)^{\dagger^Q} \equiv |\lambda\rangle$ . In addition,  $P^{-1} = \begin{pmatrix} \langle \lambda_1 |_Q \\ \langle \lambda_2 |_Q \\ \vdots \end{pmatrix}$  satisfies  $P^{-1}\hat{H}P = D$  and  $P^{-1}\hat{H}^{\dagger^Q}P = D^\dagger$ , so  $\hat{H}$  is “ $Q$ -normal”,  $[\hat{H}, \hat{H}^{\dagger^Q}] = P[D, D^\dagger]P^{-1} = 0$ . Thus the inner product  $I_Q$  makes  $\hat{H}$   $Q$ -normal. We note that  $\hat{H}$  can be decomposed as  $\hat{H} = \hat{H}_{Qh} + \hat{H}_{Qa}$ , where  $\hat{H}_{Qh} = \frac{\hat{H} + \hat{H}^{\dagger^Q}}{2}$  and  $\hat{H}_{Qa} = \frac{\hat{H} - \hat{H}^{\dagger^Q}}{2}$  are  $Q$ -Hermitian and anti- $Q$ -Hermitian parts of  $\hat{H}$ , respectively.

<sup>3</sup> Similar inner products are also studied in Refs. [15,16,25].

In Refs. [1,21,22] the future-included theory is described by using the future state  $|B(T_B)\rangle$  at the final time  $T_B$  and the past state  $|A(T_A)\rangle$  at the initial time  $T_A$ , where  $|A(T_A)\rangle$  and  $|B(T_B)\rangle$  time-develop as follows:

$$i\hbar \frac{d}{dt}|A(t)\rangle = \hat{H}|A(t)\rangle, \quad (5)$$

$$-i\hbar \frac{d}{dt}\langle B(t)| = \langle B(t)|\hat{H}, \quad (6)$$

and 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 studied. The quantity  $\langle \hat{O} \rangle^{BA}$  is called the weak value [23,24] in the real action theory (RAT). In Refs. [21,22] we investigated  $\langle \hat{O} \rangle^{BA}$ , and found that, if we regard  $\langle \hat{O} \rangle^{BA}$  as an expectation value in the future-included theory, then we obtain the Heisenberg equation, Ehrenfest’s theorem, and a conserved probability current density. Thus  $\langle \hat{O} \rangle^{BA}$  seems to play the role of an expectation value in the future-included theory.

In this letter, we adopt the proper inner product  $I_Q$  for all quantities, and hence slightly modify the final state  $\langle B(T_B)|$  as  $\langle B(T_B)| \rightarrow \langle B(T_B)|_Q$  so that the Hermitian operator  $Q$  pops out and the usual inner product  $I$  is replaced with  $I_Q$ . Our new final state  $\langle B(T_B)|$  time-develops according not to Eq. (6) but to

$$-i\hbar \frac{d}{dt}\langle B(t)|_Q = \langle B(t)|_Q \hat{H} \iff i\hbar \frac{d}{dt}|B(t)\rangle = \hat{H}^{\dagger Q}|B(t)\rangle. \quad (7)$$

Thus the normalized matrix element  $\langle \hat{O} \rangle^{BA}$  is modified into the following expression:

$$\langle \hat{O} \rangle_Q^{BA} \equiv \frac{\langle B(t)|_Q \hat{O} |A(t)\rangle}{\langle B(t)|_Q A(t)\rangle}, \quad (8)$$

where  $I_Q$  is used for both the denominator and numerator. As far as the construction of  $\langle \hat{O} \rangle_Q^{BA}$  is concerned, the shift between  $\langle B(t)|$  and  $\langle B(t)|_Q$  is just a change of notation, but, when it comes to our maximization principle, we need to normalize the initial and final states  $|A(T_A)\rangle$  and  $\langle B(T_B)|$ . There are two choices: the normalization defined with the usual inner product  $I$  or the normalization defined with the proper inner product  $I_Q$ , which we call  $Q$ -normalization. The choice of the inner product used in the normalization is not just a matter of notation, once we have chosen  $\langle \hat{O} \rangle_Q^{BA}$  as the expression of the candidate for our expectation value. That is to say, according to the choice of the inner product used in the normalization of the initial and final states, two slightly different versions could be defined. As we have explained in the introduction, each choice seems to have both advantages and disadvantages, and it is not easy to evaluate  $\langle \hat{O} \rangle_Q^{BA}$  clearly in the version with the usually normalized initial and final states, because we cannot exhaustively make use of the orthogonality of the eigenstates of the Hamiltonian  $\hat{H}$ . Therefore, we postpone the study of this version to the future, and in the following we investigate the quantity  $\langle \hat{O} \rangle_Q^{BA}$  with the  $Q$ -normalized initial and final states  $|A(T_A)\rangle$  and  $\langle B(T_B)|$ , which is much easier to study than the other version.

3. *Theorem on the normalized matrix element and its proof* We present the following theorem:

**Theorem 1.** *As a prerequisite, assume that a given Hamiltonian  $\hat{H}$  is non-normal but diagonalizable and that the imaginary parts of the eigenvalues of  $\hat{H}$  are bounded from above, and define a modified inner product  $I_Q$  by means of a Hermitian operator  $Q$  arranged so that  $\hat{H}$  becomes normal with respect to  $I_Q$ . Let the two states  $|A(t)\rangle$  and  $|B(t)\rangle$  time-develop according to the*

Schrödinger equations<sup>4</sup> with  $\hat{H}$  and  $\hat{H}^{\dagger Q}$ , respectively:  $|A(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t-T_A)}|A(T_A)\rangle$ ,  $|B(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}^{\dagger Q}(t-T_B)}|B(T_B)\rangle$ , and be normalized with  $I_Q$  at the initial time  $T_A$  and the final time  $T_B$ , respectively:  $\langle A(T_A)|_Q A(T_A)\rangle = 1$ ,  $\langle B(T_B)|_Q B(T_B)\rangle = 1$ . Next determine  $|A(T_A)\rangle$  and  $|B(T_B)\rangle$  so as to maximize the absolute value of the transition amplitude  $|\langle B(t)|_Q A(t)\rangle| = |\langle B(T_B)|_Q \exp(-i\hat{H}(T_B - T_A))|A(T_A)\rangle|$ . Then, provided that an operator  $\hat{O}$  is  $Q$ -Hermitian, i.e., Hermitian with respect to the inner product  $I_Q$ ,  $\hat{O}^{\dagger Q} = \hat{O}$ , the normalized matrix element of the operator  $\hat{O}$  defined by  $\langle \hat{O} \rangle_Q^{BA} \equiv \frac{\langle B(t)|_Q \hat{O} |A(t)\rangle}{\langle B(t)|_Q A(t)\rangle}$  becomes real and time-develops under a  $Q$ -Hermitian Hamiltonian.

Before proving the theorem, we make a couple of remarks on it. The procedure of maximizing the absolute value of the transition amplitude  $|\langle B(t)|_Q A(t)\rangle|$ , which we call the maximization principle, can be understood as an approximation to what will be with very large likelihood the result of just taking the initial state  $|A(T_A)\rangle$  and the final state  $|B(T_B)\rangle$  at random. In fact, we would like to show in a later publication that with the random states  $|A(T_A)\rangle$  and  $|B(T_B)\rangle$  we obtain approximately the same result for  $\langle \hat{O} \rangle_Q^{BA}$  as if we used the maximization principle as just stated in the theorem. The crucial point of the theorem is that  $\langle \hat{O} \rangle_Q^{BA}$ , which is taken as an average for an operator  $\hat{O}$  obeying  $\hat{O}^{\dagger Q} = \hat{O}$ , turns out to be real almost unavoidably. This is under the restriction that  $\hat{H}$  be  $Q$ -normal, i.e., normal with regard to the proper inner product  $I_Q$ , but that  $\hat{H}$  is not required to be  $Q$ -Hermitian,  $\hat{H} \neq \hat{H}^{\dagger Q}$ .

Now let us prove the above theorem by expanding  $|A(t)\rangle$  and  $|B(t)\rangle$  in terms of the eigenstates  $|\lambda_i\rangle$  as follows:  $|A(t)\rangle = \sum_i a_i(t)|\lambda_i\rangle$ ,  $|B(t)\rangle = \sum_i b_i(t)|\lambda_i\rangle$ , where  $a_i(t) = a_i(T_A)e^{-\frac{i}{\hbar}\lambda_i(t-T_A)}$ ,  $b_i(t) = b_i(T_B)e^{-\frac{i}{\hbar}\lambda_i^*(t-T_B)}$ . Since  $\langle B(t)|_Q A(t)\rangle$  is expressed as  $\langle B(t)|_Q A(t)\rangle = \sum_i R_i e^{i\Theta_i}$ , where we have introduced  $a_i(T_A) = |a_i(T_A)|e^{i\theta_{a_i}}$ ,  $b_i(T_B) = |b_i(T_B)|e^{i\theta_{b_i}}$ ,  $T \equiv T_B - T_A$ ,  $R_i \equiv |a_i(T_A)||b_i(T_B)|e^{\frac{1}{\hbar}T\text{Im}\lambda_i}$ , and  $\Theta_i \equiv \theta_{a_i} - \theta_{b_i} - \frac{1}{\hbar}T\text{Re}\lambda_i$ ,  $|\langle B(t)|_Q A(t)\rangle|^2$  is calculated as  $|\langle B(t)|_Q A(t)\rangle|^2 = \sum_i R_i^2 + 2 \sum_{i < j} R_i R_j \cos(\Theta_i - \Theta_j)$ . On the other hand, the normalization conditions are expressed as  $\sum_i |a_i(T_A)|^2 = 1$  and  $\sum_i |b_i(T_B)|^2 = 1$ , respectively.

Here we note that the imaginary parts of the eigenvalues of  $\hat{H}$  have to be bounded from above to avoid the Feynman path integral  $\int e^{\frac{i}{\hbar}S} \mathcal{D}\text{path}$  being divergently meaningless. So we assume that some of the  $\text{Im}\lambda_i$  take the maximal value  $B$ , and denote the corresponding subset of  $\{i\}$  as  $A$ . Then, since  $R_i \geq 0$ ,  $|\langle B(t)|_Q A(t)\rangle|$  can take a maximal value only under the following conditions:

$$|a_i(T_A)| = |b_i(T_B)| = 0 \quad \text{for } \forall i \notin A, \tag{9}$$

$$\Theta_i \equiv \Theta_c \quad \text{for } \forall i \in A, \tag{10}$$

$$\sum_{i \in A} |a_i(T_A)|^2 = \sum_{i \in A} |b_i(T_B)|^2 = 1, \tag{11}$$

and  $|\langle B(t)|_Q A(t)\rangle|^2$  is estimated as

$$\begin{aligned} |\langle B(t)|_Q A(t)\rangle|^2 &= \left( \sum_{i \in A} R_i \right)^2 = e^{\frac{2BT}{\hbar}} \left( \sum_{i \in A} |a_i(T_A)||b_i(T_B)| \right)^2 \\ &\leq e^{\frac{2BT}{\hbar}} \left\{ \sum_{i \in A} \left( \frac{|a_i(T_A)| + |b_i(T_B)|}{2} \right)^2 \right\}^2 = e^{\frac{2}{\hbar}BT}, \end{aligned} \tag{12}$$

<sup>4</sup> See Eqs. (5) and (7).

where the third equality is realized for

$$|a_i(T_A)| = |b_i(T_B)| \quad \text{for } \forall i \in A. \quad (13)$$

In the last equality, we have used this relation and Eq. (11). The maximization condition of  $|\langle B(t)|_Q A(t)\rangle|$  is represented by Eqs. (9)–(11) and (13). That is to say, the states to maximize  $|\langle B(t)|_Q A(t)\rangle|$ ,  $|A(t)\rangle_{\max}$  and  $|B(t)\rangle_{\max}$ , are expressed as

$$|A(t)\rangle_{\max} = \sum_{i \in A} a_i(t) |\lambda_i\rangle, \quad (14)$$

$$|B(t)\rangle_{\max} = \sum_{i \in A} b_i(t) |\lambda_i\rangle, \quad (15)$$

where  $a_i(t)$  and  $b_i(t)$  obey Eqs. (10), (11), and (13). Intuitively, it might be rather obvious that, to get the biggest transition amplitude  $|\langle B(t)|_Q A(t)\rangle|$  for states  $|A(t)\rangle$  and  $|B(t)\rangle$  normalized at the initial time  $T_A$  and the final time  $T_B$ , respectively, we should seek the eigenstates leading to the biggest increase with time development under the Schrödinger equations, i.e., with the biggest imaginary parts of the eigenvalues of  $\hat{H}$ .

We evaluate  $\langle \hat{O} \rangle_Q^{BA}$  for  $|A(t)\rangle_{\max}$  and  $|B(t)\rangle_{\max}$ . Using Eqs. (9)–(11) and (13), we obtain  $\max \langle B(t)|_Q A(t)\rangle_{\max} = e^{i\Theta_c} \sum_{i \in A} R_i = e^{i\Theta_c} e^{\frac{BT}{\hbar}}$ , and

$$\begin{aligned} \max \langle B(t)|_Q \hat{O} |A(t)\rangle_{\max} &= e^{i\Theta_c} e^{\frac{BT}{\hbar}} \sum_{i,j \in A} a_j(T_A)^* a_i(T_A) e^{\frac{i}{\hbar}(t-T_A)(\text{Re}\lambda_j - \text{Re}\lambda_i)} \langle \lambda_j |_Q \hat{O} | \lambda_i \rangle \\ &= e^{i\Theta_c} e^{\frac{BT}{\hbar}} \langle \tilde{A}(t) |_Q \hat{O} | \tilde{A}(t) \rangle, \end{aligned} \quad (16)$$

where we have introduced  $|\tilde{A}(t)\rangle \equiv e^{-\frac{i}{\hbar}(t-T_A)\hat{H}_{Qh}} |A(T_A)\rangle_{\max}$ , which is normalized as  $\langle \tilde{A}(t) |_Q \tilde{A}(t) \rangle = 1$  and obeys the Schrödinger equation

$$i\hbar \frac{d}{dt} |\tilde{A}(t)\rangle = \hat{H}_{Qh} |\tilde{A}(t)\rangle. \quad (17)$$

Thus the normalized matrix element  $\langle \hat{O} \rangle_Q^{BA}$  for  $|A(t)\rangle_{\max}$  and  $|B(t)\rangle_{\max}$  is evaluated as

$$\langle \hat{O} \rangle_Q^{BA} = \langle \tilde{A}(t) |_Q \hat{O} | \tilde{A}(t) \rangle \equiv \langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}. \quad (18)$$

Now we see that  $\langle \hat{O} \rangle_Q^{BA}$  for  $|A(t)\rangle_{\max}$  and  $|B(t)\rangle_{\max}$  has become the form of an average defined with the proper inner product  $I_Q$ . Since the complex conjugate of  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$  is expressed as  $\left\{ \langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}} \right\}^* = \left\langle \hat{O}^{\dagger Q} \right\rangle_Q^{\tilde{A}\tilde{A}}$ ,  $\langle \hat{O} \rangle_Q^{BA}$  for  $|A(t)\rangle_{\max}$  and  $|B(t)\rangle_{\max}$  is shown to be real for  $Q$ -Hermitian  $\hat{O}$ .

Next we study the time development of  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$ . We express  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$  as  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}} = \langle \tilde{A}(T_A) |_Q \hat{O}_H(t, T_A) | \tilde{A}(T_A) \rangle$ , where we have introduced the Heisenberg operator  $\hat{O}_H(t, T_A) \equiv e^{\frac{i}{\hbar}\hat{H}_{Qh}(t-T_A)} \hat{O} e^{-\frac{i}{\hbar}\hat{H}_{Qh}(t-T_A)}$ . This operator  $\hat{O}_H(t, T_A)$  obeys the Heisenberg equation

$$i\hbar \frac{d}{dt} \hat{O}_H(t, T_A) = \left[ \hat{O}_H(t, T_A), \hat{H}_{Qh} \right], \quad (19)$$

so we find that  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$  time-develops under the  $Q$ -Hermitian Hamiltonian  $\hat{H}_{Qh}$  as

$$\frac{d}{dt} \langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}} = \frac{i}{\hbar} \left\langle \left[ \hat{H}_{Qh}, \hat{O} \right] \right\rangle_Q^{\tilde{A}\tilde{A}}. \quad (20)$$

Now, for pedagogical reasons, let us suppose that  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$  time-develops under some Hamiltonian  $\hat{H}_1$  as  $\frac{d}{dt} \langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}} = \frac{i}{\hbar} [\hat{H}_1, \hat{O}]_Q^{\tilde{A}\tilde{A}}$ . The complex conjugate of this relation is given by  $\left\{ \frac{d}{dt} \langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}} \right\}^* = \frac{i}{\hbar} \left[ \hat{H}_1^{\dagger Q}, \hat{O}^{\dagger Q} \right]_Q^{\tilde{A}\tilde{A}}$ . Since  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$  is real for  $Q$ -Hermitian  $\hat{O}$ , these relations claim that  $\hat{H}_1$  has to be  $Q$ -Hermitian. Therefore, the reality of  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$  implies that it has to time-develop under some  $Q$ -Hermitian Hamiltonian. As shown in Eq. (20),  $\langle \hat{O} \rangle_Q^{\tilde{A}\tilde{A}}$  time-develops under  $\hat{H}_{Qh}$ , which is consistent with the implication. We emphasize that the maximization principle provides not only the reality of  $\langle \hat{O} \rangle_Q^{BA}$  for  $Q$ -Hermitian  $\hat{O}$  but also the  $Q$ -Hermitian Hamiltonian.

4. *Discussion* In this letter, we first reviewed the proper inner product  $I_Q$  defined with a Hermitian operator  $Q$ , which is constructed from a diagonalizing operator of a given non-normal diagonalizable Hamiltonian  $\hat{H}$ , so that the eigenstates of  $\hat{H}$  become orthogonal to each other with regard to the proper inner product  $I_Q$ , and the  $Q$ -Hermitian conjugate  $\dagger^Q$ , i.e., Hermitian conjugate with regard to  $I_Q$ . We also explained the property of the normalized matrix element  $\langle \hat{O} \rangle^{BA} = \frac{\langle B(t)|\hat{O}|A(t)\rangle}{\langle B(t)|A(t)\rangle}$  in the future-included complex action theory (CAT). Next we introduced a slightly modified normalized matrix element  $\langle \hat{O} \rangle_Q^{BA} = \frac{\langle B(t)|_Q \hat{O} |A(t)\rangle}{\langle B(t)|_Q A(t)\rangle}$ , which is defined with  $I_Q$ , and explained that two versions could be defined according to the choice of the normalization of the initial and final states  $|A(T_A)\rangle$  and  $\langle B(T_B)|$ . One is the usual normalization defined with the usual inner product  $I$ , and the other is the  $Q$ -normalization defined with the proper inner product  $I_Q$ . Assuming that a given Hamiltonian  $\hat{H}$  is non-normal but diagonalizable, and that the imaginary parts of the eigenvalues of  $\hat{H}$  are bounded from above, we presented a theorem that states that, provided that  $\hat{O}$  is  $Q$ -Hermitian, i.e.,  $\hat{O}^{\dagger Q} = \hat{O}$ , and that  $|A(t)\rangle$  and  $|B(t)\rangle$  time-develop according to the Schrödinger equations with  $\hat{H}$  and  $\hat{H}^{\dagger Q}$  and are  $Q$ -normalized at the initial time  $T_A$  and at the final time  $T_B$ , respectively,  $\langle \hat{O} \rangle_Q^{BA}$  becomes real and time-develops under a  $Q$ -Hermitian Hamiltonian for  $|A(t)\rangle$  and  $|B(t)\rangle$  such that the absolute value of the transition amplitude  $|\langle B(t)|_Q A(t)\rangle|$  is maximized. We proved the theorem by expanding  $|A(t)\rangle$  and  $|B(t)\rangle$  in terms of the eigenstates of  $\hat{H}$ . It is noteworthy that, in the future-included CAT with a priori non-normal Hamiltonian  $\hat{H}$ , we nevertheless have got a real average for  $\hat{O}$  at any time  $t$  by means of the simple expression  $\langle \hat{O} \rangle_Q^{BA}$ .

As for an emerging hermiticity, in Ref. [17] we presented a mechanism to obtain a  $Q$ -Hermitian Hamiltonian by considering a long time development. The maximization principle studied in this letter is another approach to obtaining such a  $Q$ -Hermitian Hamiltonian. We have seen that the non-hermiticity of the fundamental Hamiltonian  $\hat{H}$  has disappeared from the usually expected results of the model. It is this remarkable result of our work with non-Hermitian Hamiltonians or complex actions that allows us to consider such models to be viable. We would not have been able to see any effects of the anti-Hermitian part as far as the reality of the dynamical variables and the equations of motion are concerned. However, as earlier discussed in Ref. [1] and also seen in Eqs. (9)–(11), the anti-Hermitian part has a strong influence on the initial state, which should effectively be seen. Indeed, the maximization principle has resulted in a periodicity of the history of the universe that the initial and final states become basically the same. Such an influence would be more recognizable in a system defined with a time-dependent non-Hermitian Hamiltonian [26]. We expect the future-included CAT to have the feature that it can provide a unification of an initial condition prediction and an equation of motion. In this letter, we studied the version defined with the  $Q$ -normalized initial and final states. It would be interesting to see what kind of result we could obtain in the other version



defined with the usually normalized initial and final states, which is more difficult to study than the version studied here, because we cannot fully utilize the orthogonality of the eigenstates of the Hamiltonian  $\hat{H}$ . In the future we hope to investigate this version and to see if the reality of  $\langle \hat{O} \rangle_Q^{BA}$ , emerging Hermitian Hamiltonian, and such a periodicity are suggested or not.

Finally, assuming that the fundamental non-normal Hamiltonian  $\hat{H}$  is written in terms of Hermitian coordinate and momentum operators  $\hat{q}$  and  $\hat{p}$  as  $\hat{H} = H(\hat{q}, \hat{p})$ , we give a possible procedure<sup>5</sup> to formulate the  $Q$ -Hermitian Hamiltonian  $\hat{H}_{Qh}$  in terms of  $Q$ -Hermitian coordinate and momentum operators  $\hat{q}_Q$  and  $\hat{p}_Q$ . We also introduce a  $Q$ -Hermitian probability density operator as an example of  $Q$ -Hermitian  $\hat{O}$ , and construct a conserved probability current density. Let us begin with defining  $\hat{q}_Q$  and  $\hat{p}_Q$  by

$$\hat{q}_Q \equiv \frac{\hat{q} + \hat{q}^{\dagger Q}}{2}, \tag{21}$$

$$\hat{p}_Q \equiv \frac{\hat{p} + \hat{p}^{\dagger Q}}{2}. \tag{22}$$

Since  $Q$  depends on  $\hat{q}$  and  $\hat{p}$  via  $\hat{H}$ ,  $\hat{q}_Q$  and  $\hat{p}_Q$  could be written in terms of  $\hat{q}$  and  $\hat{p}$ , and vice versa.<sup>6</sup> Then  $\hat{H}$  would be rewritten as  $\hat{H} = H_{\text{eff}}(\hat{q}_Q, \hat{p}_Q)$ , where  $H_{\text{eff}}$  is some analytic function of  $\hat{q}_Q$  and  $\hat{p}_Q$ , and  $\hat{H}_{Qh}$  is expressed in terms of  $\hat{q}_Q$  and  $\hat{p}_Q$  as

$$\hat{H}_{Qh} = \frac{1}{2} \left( H_{\text{eff}}(\hat{q}_Q, \hat{p}_Q) + H_{\text{eff}}(\hat{q}_Q, \hat{p}_Q)^{\dagger Q} \right). \tag{23}$$

Next we define  $|q\rangle^Q$  as the eigenstate of  $\hat{q}_Q$  by  $\hat{q}_Q |q\rangle^Q = q |q\rangle^Q$  and  ${}^Q \langle q | q' \rangle^Q = \delta(q - q')$ , which suggests  $\int_{-\infty}^{\infty} dq |q\rangle^Q {}^Q \langle q | = 1$ . Similarly,  $|p\rangle^Q$  is introduced as the eigenstate of  $\hat{p}_Q$  by  $\hat{p}_Q |p\rangle^Q = p |p\rangle^Q$  and  ${}^Q \langle p | p' \rangle^Q = \delta(p - p')$ . Now, utilizing  $|q\rangle^Q$ , we define the  $Q$ -Hermitian probability density operator

$$\hat{\rho} \equiv |q\rangle^Q {}^Q \langle q | \tag{24}$$

as an example of  $Q$ -Hermitian  $\hat{O}$ , and write a  $q$ -representation of the maximizing state  $|\tilde{A}(t)\rangle$  as

$$\psi_{\tilde{A}}(q) \equiv {}^Q \langle q | \tilde{A}(t) \rangle. \tag{25}$$

Then the probability density  $\rho \equiv \langle \hat{\rho} \rangle_Q^{BA}$  is given via the maximization principle by  $\rho = \langle \hat{\rho} \rangle_Q^{\tilde{A}\tilde{A}} = |\psi_{\tilde{A}}(q)|^2$ , which obeys  $\int_{-\infty}^{\infty} dq \rho = 1$ , so we could construct a conserved probability current density

$$j(q, t) = \frac{i\hbar}{2m} \left( \frac{\partial \psi_{\tilde{A}}^*}{\partial q} \psi_{\tilde{A}} - \psi_{\tilde{A}}^* \frac{\partial \psi_{\tilde{A}}}{\partial q} \right), \tag{26}$$

which satisfies the continuity equation  $\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial q} = 0$ . In realistic cases, not only the maximizing state but also many other states contribute to the transition amplitude, while the above relations are obtained by considering only the maximizing state, which is a kind of approximation in the sense that we are ignoring the effects of the other states. But we expect that their contribution becomes

<sup>5</sup> For simplicity, we do not use the complex coordinate and momentum formalism [18] just by supposing the case where the eigenvalues  $q$  and  $p$  are essentially real. If we like, we could generalize the argument here by following Ref. [18] so that we could deal with complex  $q$  and  $p$ .

<sup>6</sup> In the harmonic oscillator model (K. Nagao and H. B. Nielsen, work in progress) defined by the Hamiltonian  $\hat{H}_{\text{ho}} \equiv \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{q}^2$  with a mass  $m$  and an angular frequency  $\omega$ , we obtain  $\hat{q}_Q = e^{i\frac{\theta}{2}} \hat{q}$  and  $\hat{p}_Q = e^{-i\frac{\theta}{2}} \hat{p}$ , where  $\theta = \arg(m\omega)$ .  $\hat{H}_{\text{ho}}$  is rewritten as  $\hat{H}_{\text{ho}} = \frac{\hat{p}_Q^2}{2m_{\text{eff}}} + \frac{1}{2} m_{\text{eff}} \omega^2 \hat{q}_Q^2$ , where  $m_{\text{eff}} = m e^{-i\theta}$ .

very small in the large  $T = T_B - T_A$  case, which we are interested in from a phenomenological point of view. The larger  $T$  we consider, the more the states with the largest positive imaginary part of energy get to dominate. Thus we have briefly given a possible procedure to formulate  $\hat{H}_{Qh}$  in terms of  $Q$ -Hermitian  $\hat{q}_Q$  and  $\hat{p}_Q$ , and also constructed a conserved probability current density for the maximizing state. However, it is not trivial at all to determine the local expression of  $\hat{H}_{Qh}$  in  $q$ -space, nor to examine the classical behavior of  $\langle \hat{O} \rangle_Q^{BA}$  explicitly. We postpone these problems to future studies.

### Acknowledgements

K.N. would like to thank the members and visitors of NBI for their kind hospitality. H.B.N. is grateful to NBI for allowing him to work at the Institute as emeritus.

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