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Statistical features of quantum evolution

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Abstract. It is shown that the integral of the uncertainty of energy with respect to time is independent of the particular Hamiltonian of the quantum system for an arbitrary pseudo-unitary (and hence $\mathcal{PT}$-) quantum evolution. The result generalizes the time–energy uncertainty principle for pseudo-unitary quantum evolutions. Further, employing random matrix theory developed for pseudo-Hermitian systems, time correlation functions are studied in the framework of linear response theory. The results given here provide a quantum brachistochrone problem where the system will evolve in a thermodynamic environment with spectral complexity that can be modelled by random matrix theory.

Keywords. $\mathcal{PT}$ symmetry; random matrix theory; time correlation functions.

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1. Introduction

During the last decade, there has been a remarkable change in our way of looking at quantum mechanics with the introduction of space-time reflection symmetry in place of Hermiticity [1]. Apart from a number of examples that have illustrated a variety of new features in the spectra of linear operators, there is a connection that has been established with pseudo-Hermiticity [2,3]. Consequently, besides the advances in pseudo-Hermitian quantum mechanics and $\mathcal{PT}$-symmetric mechanics, there have been advances in the following areas: (i) random matrix theory [3–6], (ii) exactly solvable models [7,8], (iii) applications to problems in statistical physics [6].

In this paper, we study certain geometrical aspects of quantum evolution when the system is pseudo-Hermitian or $\mathcal{PT}$-symmetric. We find very interesting generalizations of the results known in Hermitian setting. Then, we present a study on averaged time correlation function for pseudo-Hermitian quantum systems belonging to random matrix ensemble. This problem is a statistical variation of the quantum brachistochrone problem. For different ensembles, we show the long-time behaviour and make a brief comparison with the earlier work of Jain and Gaspard [9].

2. Geometry of $\mathcal{PT}$-quantum evolution

Assume that a quantum evolution of a state $|\psi(t)\rangle$ is governed by Schrödinger equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{1}$$

where H is a Hamiltonian [10]. Let us now endow the space of states $|\psi(t)\rangle$ an inner product,

$$\int \psi^{\mathcal{PT}} \psi \, \mathrm{d}\tau = \text{constant}, \tag{2}$$

where $\psi^{\mathcal{PT}}$ is the 'orthogonal' counterpart of ψ. When parity $\mathcal{P}$ and time-reversal invariance $\mathcal{T}$ are both preserved, $\psi^{\mathcal{PT}}$ will be simply the complex conjugate or Hermitian conjugate. However, when $\mathcal{P}$ and $\mathcal{T}$ are both broken, i.e. the system is $\mathcal{PT}$-symmetric, then $\psi^{\mathcal{PT}}$ is a pseudo-Hermitian conjugate. Let us write $\psi^{\mathcal{PT}}$ as $\langle\psi\eta|$ where η is acting from the right on the bra vector. Equations (1) and (2) imply that H must obey the condition of pseudo-Hermiticity,

$$H^\dagger = \eta H \eta^{-1}. \tag{3}$$

Through many examples and rigorous work (see references cited in [1] and [11,12]), it has been shown that such an operator possesses real eigenvalues if the corresponding eigenfunctions are simultaneous eigenfunctions of η; otherwise the eigenvalues occur as complex conjugate pairs with null eigenfunctions.

For an isolated system to evolve, it would always be associated with a non-zero value for uncertainty $\Delta E(t)$ defined by

$$\Delta E^2 = \langle\psi\eta|H^2|\psi\rangle - \langle\psi\eta|H|\psi\rangle^2. \tag{4}$$

This is a generalization of the definition employed in Hermitian quantum mechanics. We now show that this is connected to the geometry of the space where evolution is occurring. For this, we generalize some of the work by Aharonov and Anandan [13] by defining the projection operator $\Pi = |\psi\rangle\langle\psi\eta|$ and re-writing

$$\begin{aligned}
\left\langle \frac{\mathrm{d}\psi}{\mathrm{d}t}\eta \middle| 1-\Pi \middle| \frac{\mathrm{d}\psi}{\mathrm{d}t} \right\rangle &= \left\langle \frac{\mathrm{d}\psi}{\mathrm{d}t}\eta \middle| \frac{\mathrm{d}\psi}{\mathrm{d}t} \right\rangle - \left\langle \frac{\mathrm{d}\psi}{\mathrm{d}t}\eta \middle| \psi \right\rangle \left\langle \psi\eta \middle| \frac{\mathrm{d}\psi}{\mathrm{d}t} \right\rangle \\
&= \frac{1}{\hbar^2}\left(\langle\psi|H^\dagger\eta H|\psi\rangle - \langle\psi H^\dagger\eta|\psi\rangle\langle\psi\eta|H|\psi\rangle\right) \\
&= \frac{1}{\hbar^2}\left(\langle\psi\eta|H^2|\psi\rangle - \langle\psi\eta|H|\psi\rangle^2\right) \qquad (5) \\
&= \frac{\Delta E^2}{\hbar^2}, \qquad (6)
\end{aligned}$$

using (1) in the first step and (4) in the last step.

We can also immediately show that in the general case when H depends on time, the quantity

$$s = 2\int \frac{\Delta E(t)}{\hbar}\mathrm{d}t \tag{7}$$

is independent of the particular $H(t)$ used to transport the state. To prove this, following [13], let us make a Taylor expansion of $|\psi(t+\mathrm{d}t)\rangle$ to second order. We get

$$\begin{aligned}
|\langle\psi(t)\eta|\psi(t+\mathrm{d}t)\rangle|^2 &= \Bigg|\langle\psi(t)\eta|\psi(t) - i\frac{\mathrm{d}t}{\hbar}\langle\psi(t)\eta|H|\psi(t)\rangle \\
&\quad -i\frac{\mathrm{d}t^2}{2\hbar}\left\langle\psi(t)\eta\left|\frac{\mathrm{d}H}{\mathrm{d}t}\right|\psi(t)\right\rangle - \frac{\mathrm{d}t^2}{2\hbar^2}\langle\psi(t)\eta|H^2|\psi(t)\rangle\Bigg|^2 \\
&\quad +O(\mathrm{d}t^3) && (8)\\
&= 1 - \frac{\mathrm{d}t^2}{\hbar^2}[\langle\psi\eta|H^2|\psi\rangle - \langle\psi\eta|H|\psi\rangle^2] + O(\mathrm{d}t^3) && (9)\\
&= 1 - \frac{\mathrm{d}t^2\Delta E^2}{\hbar^2} + O(\mathrm{d}t^3), && (10)
\end{aligned}$$

which shows that $\Delta E\mathrm{d}t/\hbar$ is a purely geometric quantity. Note that the left-hand side of (5) is just the obvious generalization of Fubini–Study metric. With all these observations, we can easily write the generalized form for action [14] for arbitrary η with $\mathcal{PT}$-symmetric case as a special case to describe quantum evolutions. The expression is the same as given in [14] except the definition of the inner product.

These geometric considerations tell us that the total distance is always greater than or equal to the shortest distance connecting the initial and final quantum states. From this, we have given time–energy uncertainty principle for an arbitrary pseudo-unitary evolution.

It may be well to recall that the notion of quantum distance was first introduced by Provost and Valle [15]. The difference of their approach and the approach employed here leading to the Fubini–Study metric was clarified by Pati [16].

3. Time correlation functions

In this section, we present our study on time correlation functions. We are able to systematically obtain the analysis because of the important relations and discussions established in the earlier section. All the matrix elements employed below are consistent with the $\mathcal{PT}$-symmetric or pseudo-unitary distance function considered above.

As shown by numerous instances [17,18], these are most crucial in describing the response of a system. This is also a quantity that is closest to the measurements made by experimentalists – textbook examples being the connection of dipole–dipole correlation function and the absorption cross-section or force–force correlation function and the coefficient of kinematic viscosity. Even related to attempts at finding optimal time evolutions or what has come to be known as quantum brachistochrone problem, since these are to be realized by applying a certain field or perturbation, it is the response that needs to be found. Moreover, when we wish

to realize an evolution experimentally, the environment is thermodynamic. With all this in mind, we pose the following problem and give its solution:

Consider a system described by a Hamiltonian H which is perturbed at time $t = 0$ by an observable V such that the total Hamiltonian for times $t \geq 0$ reads as

$$H' = H + \lambda V. \tag{11}$$

Assuming that the system is in thermal equilibrium with a canonical density matrix,

$$\rho = \frac{\mathrm{e}^{-\beta H}}{\mathrm{tr}\ \mathrm{e}^{-\beta H}}, \tag{12}$$

where $T = (k\beta)^{-1}$ is temperature and k is the Boltzmann constant. The time evolution of the system at equilibrium influences the correlation function of the observable at different times. In general, n-time correlation function is written as

$$C(t_1, t_2, ..., t_n) = \mathrm{tr}\ \rho V(t_n) V(t_{n-1}) ... V(t_1). \tag{13}$$

Now, we imagine that H and V are drawn from an ensemble of Hamiltonians and observables. In particular, we assume that they belong to the same symmetry class. A rather detailed study for the Hermitian case was carried out in 1996 by Jain and Gaspard [9]. The random matrix ensemble which is pseudo-unitarily invariant was introduced in [3] where it was shown that the statistical properties of eigenvalues of pseudo-Hermitian matrices have novel properties, distinct from the known results in random matrix theory (RMT) [19].

Presently, we understand the following random matrix problems: (i) RMT for 2×2 pseudo-Hermitian case [3,4], (ii) RMT for asymmetric cyclic matrices [5], (iii) RMT for pseudo-Hermitian, cyclic blocks [6]. In the last case, there are more numerical results available than analytical results. The last problem is specially motivated by the random Ising model in two dimensions.

Among the hierarchy of correlation functions, the two-point correlation function is the most important one. In the basis of H, we can write it as

$$\begin{aligned} C(t) &= \frac{1}{Z(\beta)} \mathrm{tr}\ V(t) V(0) \\ &= \frac{1}{Z(\beta)} \mathrm{tr}\ \mathrm{e}^{i\frac{Ht}{\hbar}} V \mathrm{e}^{-i\frac{Ht}{\hbar}} V \qquad (14) \\ &= \left\langle \frac{\sum_{m,n} \mathrm{e}^{-\beta E_n + \frac{i}{\hbar} E_n t} V_{nm} \mathrm{e}^{-\frac{i}{\hbar} E_m t} V_{mn}}{\sum_n \mathrm{e}^{-\beta E_n}} \right\rangle \\ &= \left\langle \frac{Z\left(\beta - \frac{it}{\hbar}\right) Z\left(\frac{it}{\hbar}\right)}{Z(\beta)} \right\rangle v^2, \qquad (15) \end{aligned}$$

where the angular brackets denote the average over the random matrix ensemble, $\langle V_{mn} V_{nm} \rangle$ is replaced by a real constant, v^2, which is related to the variance of the distribution function employed to populate the matrix, V. In evaluating (15), we will make an approximation by replacing it as the ratio of averages. That this approximation is valid for large matrices has been argued in [9].

3.1 *Two-level pseudo-Hermitian systems*

As mentioned earlier, random matrix theory for pseudo-Hermitian Hamiltonians represented as 2×2 matrices is completely understood [3,4]. Non-trivial representations have three or four independent parameters. For the case of three independent parameters, the nearest neighbour spacing distribution near zero spacing varies as $S\log\frac{1}{S}$ whereas for the case of four independent parameters, the behaviour is $\sim\gamma S$ where γ is a constant.

Effective two-level system also are of great interest for very low temperatures where the entire Boltzmann weight concentrates on the lowest two levels. Let $E_\pm$ be the two eigenvalues so that the correlation function can be written entirely in terms of the spacing, $S = E_+ - E_-$ $(E_+ > E_-)$,

$$C(t) = v^2\left(1 + \frac{\mathrm{e}^{-i(tS/\hbar)} + \mathrm{e}^{-\beta S}\mathrm{e}^{i(tS/\hbar)}}{1+\mathrm{e}^{-\beta S}}\right). \tag{16}$$

We see that the two-point correlation function depends on the spacing, thus its ensemble average will be done with respect to the spacing distribution, $P(S)$. The long-time tail of the correlation function can be found by averaging (15) with respect to $P(S)$. We find

$$\langle C(t)\rangle \sim \frac{\hbar^2}{t^2} \tag{17}$$

at the dominant order for the general case of four parameters. The exponent on time is the same as for the time correlation function for the Gaussian orthogonal ensemble [9].

3.2 *Asymmetric cyclic matrices*

If the sizes of matrices become large, the density of eigenvalues is numerically found to be a Gaussian function of energy for asymmetric cyclic matrices [5]. We employ the following identity to obtain the partition function in terms of average density of energy levels:

$$\sum_n \mathrm{e}^{-\beta E_n} = \sum_n \int \mathrm{d}E\delta(E-E_n)\mathrm{e}^{-\beta E} = \int \mathrm{d}E\rho(E)\mathrm{e}^{-\beta E}, \tag{18}$$

where $\rho(E) = \sum_n \delta(E-E_n)$ is the average density of eigenvalues. Substituting the Gaussian form, $\mathcal{N}\mathrm{e}^{-\alpha E^2}$, we obtain immediately

$$\langle Z(\beta)\rangle = \mathcal{N}\sqrt{\frac{\pi}{4\alpha}}\exp\left(\frac{\beta^2}{4\alpha}\right) \tag{19}$$

where α sets the scale of eigenvalues.

The ensemble-averaged correlation function is

$$\langle C(t)\rangle \simeq v^2 \frac{\langle Z\left(\beta - \frac{it}{\hbar}\right) Z\left(\frac{it}{\hbar}\right)\rangle}{\langle Z(\beta)\rangle} \tag{20}$$

$$\sim \left(\cos\frac{t\beta}{2\hbar\alpha} - i\sin\frac{t\beta}{2\hbar\alpha}\right) \mathrm{e}^{-t^2/4\alpha\hbar^2}, \tag{21}$$

where in the last line we have only retained the time-dependent part. The real part crosses the t-axis first at $t_a = \pi\hbar\alpha/\beta$ which we call the first instance when the correlations become zero.

For the system with asymmetric cyclic representation, the tails in time correlation function are given as follows:

1. The spacing distribution between the complex conjugate pairs is given by a Gaussian [5],

$$P_c c(S) = \frac{2}{\pi}\mathrm{e}^{-S^2/\pi}, \tag{22}$$

and the correlation function decays as $\exp(-\pi t^2/4\hbar^2)$. Note that it does not cross the t-axis.

2. The spacing distribution between a real and a complex eigenvalue is given by [5]

$$P_r c(S) = \frac{3\sqrt{3}\pi}{16} c^2 S \exp\left(-\frac{3\pi^2}{16}c^2S^2\right) I_0\left(\frac{3\pi}{32}c^2S^2\right), \tag{23}$$

and, between any two complex eigenvalues the spacing distribution is Wigner [5]. Since both these cases exhibit linear repulsion at small spacings, the tail of the correlation will decay as t^{-2}, like (17).

4. Concluding remarks

We have shown that energy–time uncertainty principle can be given a precise meaning in pseudo-Hermitian quantum mechanics. Having stepped out of conventional quantum mechanics, we have shown that $\Delta E \mathrm{d}t/\hbar$ is a purely geometric quantity.

We have studied the time correlation functions and presented the long-time properties for two-level pseudo-Hermitian systems as well as for systems modelled in terms of asymmetric cyclic matrices. It is worthwhile to remark here that the spacing distributions found for random asymmetric cyclic matrices also extend to random matrices with cyclic blocks [6]. Thus, the results on time correlation functions are also valid there.

It is useful to note that in the limit of β becoming zero, two-time correlation functions become survival probabilities and it is in this limit that we recover the usual brachistochrone problem dealt with in earlier papers. However, these results are derived consistently within the suitably generalized framework of quantum statistical mechanics.

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