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LETTER TO THE EDITOR

Is the CPT norm always positive?

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Abstract

We give an explicit example of an exactly solvable \mathcal{PT} -symmetric Hamiltonian with unbroken \mathcal{PT} symmetry which has one eigenfunction with zero \mathcal{PT} norm. The set of its eigenfunctions is not complete in the corresponding Hilbert space and it is *non-diagonalizable*. In the case of a regular Sturm–Liouville problem any *diagonalizable* \mathcal{PT} -symmetric Hamiltonian with unbroken \mathcal{PT} symmetry has a complete set of positive \mathcal{CPT} -normalizable eigenfunctions. For nondiagonalizable Hamiltonians, a complete set of \mathcal{CPT} -normalizable functions is possible but the functions belonging to the root subspace corresponding to multiple zeros of the characteristic determinant are no longer eigenfunctions of the Hamiltonian.

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1. In recent years it has been shown that non-Hermitian Hamiltonians, in particular the \mathcal{PT} symmetric ones, may have real eigenvalues [1]. This has given rise to the possibility of constructing a complex extension of quantum mechanics [2]. Before the discovery of the Coperator [2], the main difficulty in constructing a self-consistent complex extension of quantum mechanics was the presence of negative \mathcal{PT} norms for some \mathcal{PT} -symmetric Hamiltonians. Using the CPT operation, a new norm was defined [2] and it was shown to be positive for some models. In this letter, we would like to stress that this is true only if the \mathcal{PT} norm is non-zero. Here we shall consider an explicit example of an exactly solvable \mathcal{PT} -symmetric Hamiltonian, one of whose eigenfunctions has zero \mathcal{PT} norm thus proving that such a situation may occur in a \mathcal{PT} -symmetric Hamiltonian. Further, using the fact that the \mathcal{PT} operation applied to an eigenfunction of the given Hamiltonian may only change its sign resulting in the property that the CPT operation inverts the sign of a PT norm if it is negative, we conclude that application of the CPT operation to an eigenfunction of a PT-symmetric Hamiltonian is equivalent to first going to an eigenfunction of the adjoint operator and then taking the complex conjugation provided the given solution is normalized properly. Subsequently we show that for a regular Sturm–Liouville problem the zero CPT norms may appear only if the characteristic determinant has multiple zeros. In this case the system of eigenfunctions is not complete in the corresponding Hilbert space, implying that the Hamiltonian related with such a problem is *non-diagonalizable*. We show that both for diagonalizable and non-diagonalizable Hamiltonians, one is able to define a Hilbert space with a positive CPT norm but in the latter case the basis functions corresponding to a degenerate root subspace are not eigenfunctions of the Hamiltonian.

2. In this part of our letter, we present an example of an exactly solvable \mathcal{PT} -symmetric Hamiltonian having one eigenfunction with the zero \mathcal{PT} norm.

Let us consider the following Sturm–Liouville problem in the interval $[-\pi, \pi]$:

$$\left(-\partial_x^2 + V(x) - E\right)\psi = 0\tag{1}$$

with the zero boundary conditions

$$\psi(-\pi) = \psi(\pi) = 0. \tag{2}$$

We would like to consider the following \mathcal{PT} -symmetric potential

$$V(x) = -\frac{6}{(\cos x + 2i\sin x)^2}.$$
(3)

It is not difficult to check that for a given $E = k^2 \in \mathbb{C}$, equation (1) with the potential (3) has the following solutions:

$$\psi_1 = e^{ikx} \left[2i - ki + \frac{3}{2i + \cot x} \right] \qquad \psi_2 = e^{-ikx} \left[2i + ki + \frac{3}{2i + \cot x} \right].$$
 (4)

For all $k \neq 1$ they are linearly independent since their Wronskian is $2ik(k^2 - 1)$. For k = 1 one can choose

$$\psi_1 = \frac{1}{\cos x + 2i\sin x} \qquad \psi_2 = \frac{5\sin(2x) - 4i\cos(2x) - 6x}{\cos x + 2i\sin x}.$$
 (5)

The Wronskian of these functions is equal to 4.

It is evident that the zero boundary conditions may be satisfied if and only if $\Delta = \Delta(E) = 0$ where

$$\Delta = \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix} \qquad a_{1,2} = \psi_{1,2}(-\pi) \qquad b_{1,2} = \psi_{1,2}(\pi) \tag{6}$$

is the characteristic determinant. From here for $k \neq 1$ one yields

$$(k^2 - 4)\sin(2k\pi) = 0.$$
 (7)

This corresponds to the purely real spectrum $k = k_n = n/2$

$$E_n = n^2/4$$
 $n = 1, 3, 4, 5, \dots$ (8)

It may be pointed out that all roots of equation (7) are simple except for $E = k^2 = 4$ which is a double root and it will be shown that this result has important consequences. For k = 1, $\Delta \neq 0$ meaning that E = 1 (n = 2) is not a spectral point. We would like to note that the whole spectrum is simple (i.e. there is only one eigenfunction for every eigenvalue) including the point E = 4 and the existence of the double root of the equation $\Delta(E) = 0$ is not related with the (non-)degeneracy of the eigenvalue E = 4. This can be easily seen from (4). For instance at $k = 4 \psi_1(\pm \pi) = 0$ but $\psi_2(\pm \pi) \neq 0$.

The eigenfunctions are

$$\psi_n = \frac{\left[(16 - n^2)\cos x - 2i(n^2 - 4)\sin x\right]\sin\left[\frac{n}{2}(\pi + x)\right] - 6n\sin x\cos\left[\frac{n}{2}(\pi + x)\right]}{\cos x + 2i\sin x}.$$

They are \mathcal{PT} orthogonal (we recall that $\mathcal{PT} \psi_n(x) = \psi_n^*(-x)$), and it is not difficult to find their \mathcal{PT} norm, so

$$\int_{-\pi}^{\pi} \psi_n(x) [\mathcal{PT} \, \psi_m(x)] \, \mathrm{d}x = \pi \, (-1)^{n+1} (n^2 - 4) (n^2 - 16) \delta_{nm} \qquad n \neq 2. \tag{9}$$

Thus we see that the \mathcal{PT} norm of ψ_4 is null. This means that if one defined the \mathcal{CPT} inner product by redefining the \mathcal{PT} -inner product in a way that the vectors with a negative \mathcal{PT} norm would become the vectors with a positive \mathcal{CPT} norm (in our case it would be $\|\psi_n\|_{\mathcal{CPT}}^2 = \pi (n^2 - 4)(n^2 - 16), n = 1, 4, 5, ...$ and $\|\psi_3\|_{\mathcal{CPT}}^2 = 35\pi$), the vectors with the zero \mathcal{PT} norm (ψ_4 in our example) would still remain as vectors with the zero \mathcal{CPT} norm and the metric of such a space would be neither negative nor positive. Another interesting observation is $\mathcal{PT} \psi_n = (-1)^{n-1} \psi_n, n = 1, 3, 4...$, but since the vector with n = 2 is missing, the \pm signs do not alternate for two adjacent points of the spectrum n = 1 and n = 3.

An important property of a spectral problem such as the one given in (1–3) is that the set of eigenfunctions $\{\psi_n\}$ is not complete in $L^2(-\pi, \pi)$. Nevertheless, it is remarkable that one can find the missing functions and enlarge the set of eigenfunctions till a set complete in $L^2(-\pi, \pi)$ and these missing functions are related just with the multiple roots of the equation $\Delta(E) = 0$. We shall now show that in our particular case the single missing function is related not with the missing value of n = 2 but with the eigenfunction

$$b_4 = \frac{-24 \,\mathrm{e}^{2\mathrm{i}x} \sin x}{\cos x + 2\mathrm{i}\sin x} \tag{10}$$

corresponding to the double root of the equation $\Delta(E) = 0$. To find this function we introduce a special solution $\psi(x, k)$, $E = k^2$ of the spectral problem (1)–(2) such that $\psi(-\pi, k) = 0$ fixing the normalization by the condition $\psi'(-\pi, k) = 1$. (By the prime, we denote the derivative with respect to x.) It can easily be found with the help of the solutions (4) to see that

$$\psi(\pi,k) = \frac{(k^2 - 4)\sin(2k\pi)}{k(k^2 - 1)} \tag{11}$$

and the equation $\psi(\pi, k) = 0$ has exactly the same roots as $\Delta(E) = 0$ (see equation (7)). In particular all roots are simple except for k = 2 which is a double root. (Note that $\psi(x, \frac{n}{2})$ may differ from ψ_n only by a constant factor.) For this reason its derivative with respect to $k, \dot{\psi}(x, k) \equiv \partial \psi(x, k)/\partial k$, at k = 2

$$\dot{\psi}(x,2) = \frac{1}{12} [12i\pi - 7 + 12ix + 8e^{-2ix} - e^{-4ix}]\psi(x,2)$$
(12)

satisfies the zero boundary conditions, $\dot{\psi}(\pm \pi, 2) = 0$ also. It is evidently linearly independent with the function (10) and \mathcal{PT} orthogonal with ψ_n , n = 1, 3, 5, 6, 7... which may be checked by the direct calculation meaning that it is linearly independent with the set of eigenfunctions $\{\psi_n\}$. It follows from equation (1) that it satisfies the inhomogeneous equation

$$\left[-\partial_x^2 + V(x) - 4\right]\dot{\psi}(x, 2) = 4\psi(x, 2).$$
(13)

The function $\psi(x, 2)$ is called *associated function* with the eigenfunction $\psi(x, 2)$ (see e.g. [4, 5]). It can be proven (see e.g. [5], theorem 1.3.1) that the set $\{\psi_n\}, n = 1, 3, 4, 5...$ supplemented with $\dot{\psi}(x, 2)$ or equivalently with

$$\varphi_4 = \frac{12ix \ e^{2ix} - e^{-2ix} + 8}{\cos x + 2i\sin x} \sin x \tag{14}$$

is complete in $L^2(-\pi, \pi)$. One can note that ψ_4 and either φ_4 or $\dot{\psi}(x, 2)$ form a basis in the two-dimensional root subspace \mathcal{L}_4 corresponding to the energy E = 4 and they both satisfy the homogeneous equation

$$\left[-\partial_x^2 + V(x) - 4\right]^2 \psi(x) = 0 \qquad \psi(-\pi) = \psi(\pi) = 0.$$
(15)

For ψ_4 this follows from (1) and for $\dot{\psi}(x, 2)$ one should also take into account equation (13). Let us introduce a short notation to the integral

$$\int_{-\pi}^{\pi} \psi_n(x) \psi_m(x) \, \mathrm{d}x \equiv (\psi_n, \psi_m).$$

Then by the direct calculation one can find that $(\varphi_4, \varphi_4) = -44\pi$ and $(\varphi_4, \psi_4) = -96\pi$. Now in the root subspace \mathcal{L}_4 one can choose the basis we denote ξ_2 and ξ_3 such that $(\xi_n, \xi_m) = \delta_{nm}, n, m = 2, 3$,

$$\xi_2 = i\psi_4 \sqrt{(\varphi_4, \varphi_4)}/(\varphi_4, \psi_4) - i\varphi_4/\sqrt{(\varphi_4, \varphi_4)}$$
 $\xi_3 = \varphi_4/\sqrt{(\varphi_4, \varphi_4)}$

and renormalize all other basis functions

$$\xi_n = \psi_n / \sqrt{\pi (n^2 - 4)(n^2 - 16)}$$
 $n = 1, 5, 6, 7, \dots$ $\xi_4 = \psi_3 / \sqrt{-35\pi}$

So, the new basis $\{\xi_n\}$ has the following properties:

$$\mathcal{PT}\xi_n = (-1)^{n-1}\xi_n \qquad (\xi_n, \xi_m) = \delta_{nm}$$
$$\left(-\partial_x^2 + V(x) - E_n\right)^2 \xi_n = 0 \qquad \xi_n(\pm \pi) = 0$$

with $E_n = n^2/4$ for $n = 1, 5, 6, 7, ..., E_2 = E_3 = 4$ and $E_4 = 9/4$ which readily follow from the properties of the functions ψ_n and φ_4 .

Before ending this section we would like to point out that the zero \mathcal{PT} norm of ψ_4 is not accidental but is due to the fact that the root k = 2 of the equation $\psi(\pi, k) = 0$ is a double root. Indeed, since $\psi(x, k)$ satisfies equation (1) one has

$$(k^2 - \tilde{k}^2)\psi(x,k)\psi(x,\tilde{k}) = \frac{\mathrm{d}}{\mathrm{d}x}[\psi'(x,k)\psi(x,\tilde{k}) - \psi(x,k)\psi'(x,\tilde{k})]$$

from which it follows that at $\tilde{k} = n/2$

$$\int_{-\pi}^{\pi} \psi(x,k)\psi(x,\frac{n}{2}) \,\mathrm{d}x = \frac{1}{\frac{n^2}{4} - k^2} \psi'(\pi,\frac{n}{2})\psi(\pi,k).$$
(16)

Noting that $\psi'(\pi, \frac{n}{2}) = (-1)^n \neq 0$ and taking into account (11) we conclude that for k = 2 (n = 4), $(\psi_4, \psi_4) = 0$, and for $k \neq 2$, $(\psi_n, \psi_n) \neq 0$, n = 1, 3, 5, 6, 7, ... This is a property which does not depend on a particular choice of the potential V(x) and takes place for any eigenfunction (if present) of the boundary value problem (1)–(2) with the simple spectrum corresponding to a double root of the equation $\psi(\pi, k) = 0$. In particular, any such eigenfunction of a \mathcal{PT} -symmetric Hamiltonian corresponding to a regular Sturm–Liouville problem has zero \mathcal{PT} norm.

So, from this example we see that the set of eigenfunctions of the problem (1)–(3) is not complete but may be completed. In the next section, we shall see that such a situation though unacceptable from the quantum mechanical viewpoint is usual in the theory of ordinary linear differential operators and our example presents an elementary illustration of known theorems [4, 5]. This is related to the fact that in the usual quantum mechanics, one always deals with *diagonalizable* Hamiltonians while in complex quantum mechanics this is not always so.

3. Here we first recall some facts from the theory of ordinary linear differential operators [4, 5] and then show how a new (*dynamical*) inner product in the space $L^2(-\pi, \pi)$ can be defined. Everywhere we shall assume that the spectrum of the boundary value problem of type (1)–(2) is real as it is in our example.

I. A boundary value problem similar to that given by (1)–(2) with a complex-valued function V(x) defines a non-selfadjoint operator H in the Hilbert space $L^2(-\pi,\pi)$ with the dense domain of definition consisting of all twice differentiable functions vanishing at $x = \pm \pi$. The adjoint problem obtained from (1)–(2) by replacing V(x) with its complex

conjugate $V^*(x)$ defines the operator H^+ which is Hermitian adjoint to H. Since H has a real spectrum, H^+ has the same spectrum and the known bi-orthogonality condition between the eigenfunctions of H, $\psi_n(x)$, and those of H^+ , $\tilde{\psi}_{n'}(x) = \psi_{n'}^*(x)$, has the form

$$\langle \widetilde{\psi}_{n'} | \psi_n \rangle \equiv (\psi_{n'}, \psi_n) = \int_{-\pi}^{\pi} \psi_{n'}(x) \psi_n(x) \,\mathrm{d}x = 0 \qquad n \neq n'.$$
(17)

By the angle brackets we denote the usual inner product in $L^2(-\pi, \pi)$ and the round brackets define a new inner product to be defined later (see below).

II. The spectrum of *H* coincides with the zeros of the determinant $\Delta(E)$ given by (6) or equivalently with the solutions of the equation $\psi(\pi, k) = 0$ where $\psi(x, k)$ is a solution vanishing at $x = -\pi$ for all *k*. If *H* is Hermitian $\Delta(E)$ has only simple zeros. For complex potentials the equation $\Delta(E) = 0$ may have multiple zeros as in the example above. The situation with multiple zeros is an extension to differential equations of the property known in the linear algebra for a non-diagonalizable matrix which can nevertheless be reduced to a canonical Jordanian form. Using this analogy one may call such Hamiltonians *non-diagonalizable*. The set of their eigenfunctions is not complete in $L^2(-\pi, \pi)$ but may be completed. Otherwise the Hamiltonian is called *diagonalizable* (cf [6]). For a diagonalizable Hamiltonian (ψ_n, ψ_n) $\neq 0 \forall n$, the set { ψ_n } is complete in $L^2(-\pi, \pi)$ and they can always be normalized such that

$$(\psi_n, \psi_n) = \int_{-\pi}^{\pi} \psi_n^2(x) \, \mathrm{d}x = 1.$$
(18)

For the case when a continuous spectrum is present, the concept of diagonalizability should be examined more carefully.

III. In conventional quantum mechanics the property that self-adjoint operators have a complete set of eigenfunctions in the corresponding Hilbert space plays a crucial role. Now we would like to discuss the role of this property in the case of non-selfadjoint operators. In particular, the following theorem ([4], theorem 4, chapter II section 3) is extremely useful:

Theorem 1. Let operator H be generated by regular boundary conditions. Let all its eigenvalues be simple zeros of the function $\Delta(E)$ defined in (6). Then any f(x) belonging to the domain of definition of H can be developed over its eigenfunctions in the uniformly convergent series

$$f(x) = \sum_{n=1}^{\infty} a_n \psi_n(x) \tag{19}$$

$$a_n = \int_{-\pi}^{\pi} f(\mathbf{y}) \widetilde{\psi}_n^*(\mathbf{y}) \,\mathrm{d}\mathbf{y} \tag{20}$$

where $\psi_n(x)$, $\tilde{\psi}_n(x)$ are eigenfunctions of H and H^+ corresponding to the eigenvalues E_n and E_n^* respectively.

Remark. It is not explicitly stated in this theorem but the eigenfunctions are assumed to be normalized to satisfy equation (18).

We refer the reader to the book [4] for the general definition of regular boundary conditions of a boundary value problem for an *n*th order differential operator. For our purposes it is sufficient to note that *non-degenerate* boundary conditions used by Marchenko [5] are regular. They are specified as the conditions for which the characteristic function $\Delta(E)$ is not constant for the zero potential V(x) = 0. Evidently the boundary conditions given in (2) satisfy this property. At first glance it would seem that this is exactly the result that one needs in quantum mechanics. But for a self-adjoint Hamiltonian a stronger theorem is valid, namely, the set of its eigenfunctions is complete in $L^2(-\pi, \pi)$. This means that for any element from $L^2(-\pi, \pi)$ the corresponding Fourier series converges in the squared mean. A similar statement takes place for complex Hamiltonians also but under some additional restriction imposed on the boundary conditions. We will not go into further detail but refer the interested reader to the book by Naimark [4]. We only note that the non-degenerate boundary conditions by Marchenko and in particular conditions (2) have this property and the eigenfunctions of the boundary value problem (1)–(2) form Riesz basis known also as a basis equivalent to an orthonormal basis in which case a counterpart of the Parseval equality can be formulated for any element from $L^2(-\pi, \pi)$. The completeness condition for the set of eigenfunctions of *H* normalized according to (18) in the space $L^2(-\pi, \pi)$ has almost the usual form, only the complex conjugation is absent

$$\sum_{n=1}^{\infty} \psi_n(x)\psi_n(y) = \delta(x-y).$$
(21)

Once the property that the system of eigenfunctions of H is complete in $L^2(-\pi, \pi)$ is established, we can define a new Hilbert space as follows. First we define a new positive definite sesquilinear functional over the linear hull (lineal) \mathcal{L} of all finite linear combinations of the solutions of the boundary value problem (1)–(2) and then close this space with respect to the norm generated by this functional. For that we note that together with equation (1), we have the adjoint boundary value problem defined by the differential equation $(H^+ - E)\tilde{\psi} = 0$ with the boundary conditions (2). In general, the lineal \mathcal{L}^* of corresponding solutions of the latter equation is different from \mathcal{L} although they both are included in $L^2(-\pi, \pi)$. According to the left-hand side of equation (17) just elements from \mathcal{L}^* participate in the biorthogonality condition. Therefore, to be able to use this equation while defining the new inner product for elements from \mathcal{L} we have to map lineal \mathcal{L}^* onto \mathcal{L} . We realize this mapping first between the basis functions, $\psi_n \leftrightarrow \tilde{\psi}_n = \psi_n^*$ and then continue it by linearity to the whole spaces \mathcal{L}^* and $\mathcal{L}: \psi_n + \psi_m \leftrightarrow \tilde{\psi}_n + \tilde{\psi}_m = \psi_n^* + \psi_m^*, c\psi_n \leftrightarrow c\tilde{\psi}_n = c\psi_n^*$. Once the correspondence $\psi \leftrightarrow \tilde{\psi}$, is established $\forall \psi \in \mathcal{L}, \forall \tilde{\psi} \in \mathcal{L}^*$, one can define in \mathcal{L} a positive definite sesquilinear functional, (\cdot, \cdot) , (the new inner product) as follows:

$$(\psi, \varphi) = \langle \widetilde{\psi} | \varphi \rangle \qquad \psi, \varphi \in \mathcal{L} \qquad \psi \to \widetilde{\psi} \in \mathcal{L}^*.$$
 (22)

It is evident that because of the bi-orthonormality conditions (17), (18) the basis ψ_n becomes orthonormal with respect to the new inner product. Moreover, for any ψ of the form $\psi = \sum_{k=1}^{n} c_k \psi_k \neq 0$ the value $(\psi, \psi) = \sum_{k=1}^{n} |c_k|^2$ being positive can be associated with the squared norm, so that $\|\psi\| = (\psi, \psi)^{1/2}$. Now the closure of the space \mathcal{L} with respect to this norm gives us the desired Hilbert space \mathcal{H} . (The sesquilinear functional (22) should be extended from the lineal \mathcal{L} to the whole space \mathcal{H} by continuity.)

For multiple zeros of the function $\Delta(E)$ a complete set in $L^2(-\pi, \pi)$ can also be found but now together with the eigenfunctions one has to find their associated functions. For every eigenfunction $\psi(x, E_m)$ corresponding to a simple eigenvalue E_m with p_m being the order of the zero E_m of the function $\Delta(E)$ the chain of associated functions is defined as $[4, 5]: [\partial^n \psi(x, E)/\partial E^n]_{E=E_m}, n = 1, \dots, p_m - 1$. The eigenfunctions together with the set of corresponding associated functions form for the given value of the energy a root subspace. The completeness condition of the set of eigenfunctions enlarged by corresponding associated functions was first studied by Keldysh [7, 4]. It is clear that in every p_m -dimensional root subspace one can choose a basis ξ_{m_n} such that $(\xi_{m_n}, \xi_{m_{n'}}) = \delta_{m_n,m_{n'}}$ and the complete set of eigenfunctions and associated functions may be transformed into a set orthonormal with respect to the inner product (\cdot, \cdot) . Since our construction of the Hilbert space \mathcal{H} is based on the orthonormality of the basis set $\{\psi_n\}$ with respect to this inner product, it is valid for the set $\{\xi_{m_n}\}$ also.

4. The properties of \mathcal{PT} -symmetric *diagonalizable* Hamiltonians with unbroken \mathcal{PT} symmetry, a real spectrum and the eigenfunctions normalized according to (18), permit us to state that

- (a) the CPT-inner product defined in [2] coincides with the inner product (·, ·) introduced above. This follows from the fact that they apparently coincide on solutions of the boundary value problem (1)–(2) which form a basis in L²(-π, π) and both are sesquilinear. We infer, hence, that any such Hamiltonian has positive CPT-normalizable eigenfunctions;
- (b) CPT completeness condition (see [2]) is equivalent to the usual completeness condition for a non-selfadjoint Hamiltonian in the space $L^2(-\pi, \pi)$ given by (21);
- (c) CPT extension of quantum mechanics for such Hamiltonians should follow the same lines already reported in [2] but as long as the situation with the continuous spectrum is unclear this extension is incomplete.

We hope that similar extension is possible for Hamiltonians with continuous spectrum also. This optimism is based on the fact that for this case a counterpart of the Parceval equality also exists [8] but the lack of a counterpart of the Riesz basis does not permit us to form a definite conclusion.

For non-diagonalizable Hamiltonians with a simple spectrum, the situation is such that for a given non-degenerate value of the energy there exist at least two different functions, one is eigenfunction while the other is its associated function. As our example shows, in this case it is still possible to construct a complete set orthonormal with respect to an appropriately defined inner product but the functions belonging to the same root subspace are not eigenfunctions of the Hamiltonian anymore. Moreover, if the basis functions have a definite \mathcal{PT} parity the \mathcal{CPT} inner product should coincide with the inner product (\cdot, \cdot) and, hence, the basis is positive \mathcal{CPT} normalizable. We leave open the question of whether the quantum mechanics may be extended to this case.

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