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Plea for a unitary time reversal operator

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Abstract:	We take a fresh look at the time reversal operator by examining the arguments in favor of the anti-unitarity of this operator and by proposing counter-arguments in order to validate the possibility for this operator to be unitary.
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Highlights :

- A new nature of time reversal is introduced
- It allows the existence of negative energy states (sources of intensive studies in cosmology)
- It is compatible with the invariance of the fundamental results of quantum mechanics
- Extensions are possible in field theory and in Lie groups and algebras developments

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Plea for a unitary time reversal operator

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Abstract

We take a fresh look at the time reversal operator by examining the arguments in favor of the anti-unitarity of this operator and by proposing counter-arguments in order to validate the possibility for this operator to be unitary.

Keywords: Time reversal operator, discrete symmetries, non-relativistic quantum mechanics

1. Introduction

Since Wigner's symmetry representation theorem [1], we know that a symmetry operator i.e. an operator preserving transition probabilities, is necessarily unitary or anti-unitary.
As a reminder, a unitary operator T is such that

$$T^\dagger T = I \tag{1}$$

($T^\dagger$ being the adjoint of T).
It also ensures linearity

$$T(c_1 |\psi_1\rangle + c_2 |\psi_2\rangle) = c_1 T |\psi_1\rangle + c_2 T |\psi_2\rangle, \quad c_1, c_2 \in \mathbb{C}. \tag{2}$$

Such an operator preserves the scalar product (and thus the probabilities)

$$\langle\psi_1|\psi_2\rangle = \langle T\psi_1|T\psi_2\rangle. \tag{3}$$

An anti-unitary operator returns the complex conjugate of this scalar product (but therefore also preserves the probabilities)

$$\langle\psi_1|\psi_2\rangle^* = \langle T\psi_1|T\psi_2\rangle. \tag{4}$$

It is thus anti-linear

$$T(c_1 |\psi_1\rangle + c_2 |\psi_2\rangle) = c_1^* T |\psi_1\rangle + c_2^* T |\psi_2\rangle. \tag{5}$$

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This theorem has since been generalized under the name of Uhlhorn's theorem [2]. The latter is based on a less restrictive assumption: it is sufficient to request that

$$\langle\psi_1|\psi_2\rangle = 0 \iff \langle T\psi_1|T\psi_2\rangle = 0 \tag{6}$$

to ensure that T is either unitary or anti-unitary.

In any case, the conclusion is the same: a symmetry operator is necessarily unitary or anti-unitary.

When the symmetry concerns continuous transformations (translations, rotations,...), the choice is obvious: the operator is necessarily unitary. The reason is simple. For these transformations, we have:

$$U(a)U(b) = U(c).$$

Now, a product of two unitary operators as well as a product of two anti-unitary operators is automatically unitary. This fixes univocally the unitarity of U.

The same is not true for discrete symmetries, of which time reversal is a part. In this case, the nature of the symmetry operator is left to the choice of the physicists and, as far as time reversal is concerned, this choice is (almost) unanimously fixed as being the anti-unitarity.

We discuss here this choice with its advantages and disadvantages and highlight another option: that of the unitarity of the time inversion T.

To do this, we briefly review the reasons for this choice in connection with the elements of classical mechanics in Section 2. We then point out, in Section 3, three arguments, frequently found in the standard literature, for why T should be anti-unitary. To these three arguments, we oppose counter-arguments arguing for the unitarity of T. We also show that considering T as a unitary operator has the same effect as applying the complex rotation method. This will be achieved in Section 4 as well as the introduction of a new inner product. We finally conclude by listing in a table the characteristics of the two options.

2. A little detour through classical mechanics

The time inversion in classical mechanics is defined by

$$t \mapsto -t \tag{7}$$

and its impact on the variables of the phase space is

$$\vec{r} \mapsto \vec{r}, \quad \vec{v} = \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} \mapsto -\vec{v} \tag{8}$$

It is customary to consider indifferently the velocity $\vec{v}$ or the momentum $\vec{p}$ to characterize the phase space. Yet, in the case at hand i.e. the consideration of time reversal, the difference is going to be crucial. Indeed, there are as many "definitions" of momentum in classical mechanics as there are Lagrangians or Hamiltonians, whereas there is only one definition for velocity.

For example the Lagrangian of classical electrodynamics is given by

$$L = T - V = \frac{1}{2} m \vec{v} \cdot \vec{v} - q\phi + q \vec{v} \cdot \vec{A} \tag{9}$$

(q is the electric charge, ϕ the scalar potential, and $\vec{A}$ the vector potential). Momenta are defined by

$$\vec{p} = \frac{\partial L}{\partial \vec{v}}, \tag{10}$$

which gives rise here to

$$\vec{p} = m\vec{v} + q\vec{A}. \tag{11}$$

The only way to ensure that the momentum changes sign under time reversal is thus to force the potential vector to change sign, too. However, if we consider f.i. the (frequently used) case of a constant magnetic field

$$\vec{B} = B\vec{e}_z, \quad B = constant, \tag{12}$$

and the associated vector potential

$$\vec{A} = -\frac{B}{2}\vec{e}_x + \frac{B}{2}\vec{e}_y, \tag{13}$$

we see clearly that this constraint of change of sign does not make sense.

Consequently, and in agreement with Albert [3], we conclude that the momentum does not necessarily change sign under time inversion: in some cases (the free case, for instance), it does and in other cases (as recalled above), it doesn't.

3. The quantum time reversal operator: unitary or anti-unitary?

As mentioned in the Introduction, it is commonly agreed that T is anti-unitary. However some discordant voices are raised to oppose this choice. For example, Albert [3] and Callender [4] claim that time reversal has to be defined just as the classical time reflection (7) while the standard choice is

$$\psi(\vec{r}, t) \mapsto T\psi(\vec{r}, -t), \tag{14}$$

($\psi(\vec{r}, t)$ is the solution of the Schrödinger equation). Obviously, this is equivalent to considering T as the (unitary) identity operator. Other unitary proposals for T can be found in [5] and [6] when the Dirac equation/field is under study.

Despite these few proposals, the majority of physicists are convinced that only the anti-unitarity of T is a valid option. Let us examine their arguments and see what these arguments become in the light of the unitarity of time reversal.

3.1. *Argument 1: the quantum momentum must change sign, like its classical version*

If we accept this point and if we remember that the momentum has been quantized through

$$\vec{p} = -\mathrm{i}\hbar\vec{\nabla}, \tag{15}$$

and as neither the Dirac constant nor the gradient can be transformed by T, we are left with one option only: change the sign of i, and this is precisely the role of an anti-unitary operator. Moreover, this ensures the invariance of the fundamental relation of quantum mechanics (we write with bold letters the quantities which change sign under the action of T)

$$[x_j, \mathbf{p}_k] = \mathbf{i}\hbar\delta_{jk}. \tag{16}$$

Let's come to the counter-argument. As we have seen in the first section, the classical momentum does not necessarily change sign. So why should the quantum momentum do so? It is also self-consistent to ask for the status-quo for the momentum and the invariance for the relation (16) since, as well the left as the right member, do not undergo any change of sign with a unitary temporal inversion.

Close to this point, we find Callender's [4] saying that the Ehrenfest theorem implies

$$\frac{\mathrm{d}\langle\vec{r}\rangle}{\mathrm{d}t} = \frac{1}{m}\langle\vec{p}\rangle, \tag{17}$$

and, consequently, the mean value of $\vec{p}$ has to change sign. Besides the fact that Callender himself would say a few years later [7] that he was not totally convinced by this argument, we could mention that, once again, this point is not valid anymore for other choices of Hamiltonians. For instance, the Pauli Hamiltonian leads to

$$\frac{\mathrm{d}\langle\vec{r}\rangle}{\mathrm{d}t} = \frac{1}{m}\left\langle\vec{p} - q\vec{A}\right\rangle, \tag{18}$$

which has no reason to be invariant under T.

Ehrenfest's theorem is therefore not invariant under time inversion, whether T is unitary or anti-unitary (and it is clear that to ask for the invariance of all relations is a challenge, and a useless one at that). Nevertheless, we will find back the results associated with anti-unitary T i.e. the invariance of the Ehrenfest theorem in some cases, by passing to unitarity provided we generalize the inner product. This will be done in section 4.

On the contrary, the fundamental relation (16) of quantum mechanics is invariant, whether T is anti-unitary or unitary.

3.2. *Argument 2: a unitary time reversal operator leads to negative energies*

In 2016, Robert showed [8] (and we can find f.i. similar developments in [9]) that, given the following three assumptions on the Hamiltonian H

$$\begin{cases} \langle\psi|H|\psi\rangle \geq 0, \ \forall\psi \\ H \neq 0 \\ T\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht}T^{-1} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht} \end{cases},$$

then T is necessarily anti-unitary.

The second assumption is trivial and the third one comes from

$$T e^{\frac{i}{\hbar} H t} T^{-1} = e^{T \frac{i}{\hbar} H t T^{-1}}, \tag{19}$$

implying

$$T \, iH \, T^{-1} = -iH. \tag{20}$$

If T is unitary, then it means that it has to anticommute with H

$$HT = -TH. \tag{21}$$

Now, T as a symmetry, must preserve the scalar product. It follows that

$$\langle \psi | H \psi \rangle = \langle T\psi | TH\psi \rangle = -\langle T\psi | HT \; \psi \rangle . \tag{22}$$

And there we are faced with a state $T|\psi\rangle$ which is of negative energy since $\langle \psi | H\psi \rangle \geq 0$, by assumption. Roberts therefore eliminates the fact that T is unitary since this contradicts his first assumption.

Let's come to the counter-argument. Nothing says that all energies must be positive... In fact, there is even more and more evidence to say that particles of negative masses ([10–14]) (equivalent to negative energies in the relativistic context) are one of the best candidates to define the nature of dark matter ([15, 16]). If this hypothesis holds true in the years to come, the time reversal must necessarily be unitary.

3.3. *Arg,ument 3: the invariance of the Schrödinger equation*

If we follow the tradition of having T anti-unitary, the Schrödinger equation

$$\mathbf{i}\hbar \frac{\partial \psi}{\partial \mathbf{t}} = -\frac{\hbar^2}{2m} \Delta \psi + V\psi \tag{23}$$

is indeed invariant while the unitary version seems to lead to a variable one.

To better understand, we must go back to the origins and thus to the set of six papers published by Schrödinger in 1926 [17]. The starting point of Schrödinger was to find an equation, similar to that of the waves, whose solutions would be of the plane wave type

$$\psi_1 = A_1 e^{-\frac{i}{\hbar}(Et - \vec{p} \cdot \vec{x})}, \quad \psi_2 = A_2 e^{-\frac{i}{\hbar}(Et + \vec{p} \cdot \vec{x})}, \quad A_1, A_2 \in \mathbb{C}. \tag{24}$$

After a first proposal, he highlighted what he put forward as the (real) equation of non-relativistic quantum mechanics

$$(\Delta - \frac{2m}{\hbar^2} V)^2 \psi(\vec{r}, t) + \frac{4m^2}{\hbar^2} \frac{\partial^2 \psi(\vec{r}, t)}{\partial t^2} = 0, \tag{25}$$

or, by the usual factorization of the wavefunction,

$$\left(\left(\Delta - \frac{2m}{\hbar^2} V \right)^2 - \frac{4m^2}{\hbar^2} E^2 \right) \phi(\vec{r}) = 0. \tag{26}$$

This (fourth-order) equation is obviously invariant under time reflection but also admits solutions with negative energies. It is particularly easy to convince oneself of this by considering the example of the one-dimensional harmonic oscillator for which

$$V = \frac{1}{2}m\omega^2 x^2, \tag{27}$$

and

$$\left(\left(\Delta - \frac{m^2\omega^2}{\hbar^2}x^2\right)^2 - \frac{4m^2}{\hbar^2}E^2\right)\phi(\vec{r}) = 0. \tag{28}$$

Indeed the usual solutions arise

$$\phi(x) = \sqrt[4]{\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}}\,\mathrm{e}^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \tag{29}$$

but with positive as well as negative energies[2]

$$E = \pm\hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots \tag{30}$$

Given the technical difficulties that a fourth-order equation could cause, Schrödinger then proposed a final version that would simplify the calculations

$$\left(\Delta - \frac{2m}{\hbar^2}V \pm \frac{2\mathrm{i}m}{\hbar}\frac{\partial}{\partial t}\right)\psi(\vec{r}, t) = 0 \tag{31}$$

(see Eq. (32) of [19]).

The sign ambiguity in front of the time derivative clearly leaves room for both negative and positive energies and thus for the unitarity of T (see argument 2). This means that the *complete* Schrödinger equation, with the two possible signs in front of the time derivative, is invariant under unitary time inversion. This equation can take a matrix form

$$\mathrm{i}\hbar\sigma_3\frac{\partial\psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi(\vec{r}, t) + V\psi(\vec{r}, t), \tag{32}$$

(σ_3 is the usual —diagonal— Pauli matrix) or, equivalently

$$\mathrm{i}\hbar\frac{\partial\psi(\vec{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta + V\right)\sigma_3\psi(\vec{r}, t). \tag{33}$$

As a unitary time reversal operator has to anticommute with H (see Eq. (21)), it can be realized for instance through

$$T = \sigma_2, \tag{34}$$

up to a constant. The action of this operator is to reverse the components of the ψ, i.e., to reverse the signs of the energies.

[2] This result has also been demonstrated from the standard Schrödinger equation [18].

Let us also mention that the equation (33) has some common points with the supersymmetric version of quantum mechanics [20] such as two components for the Hamiltonian, one of them leading to negative energies, or the presence of an anticommutation relation (Eq. (21)). However, there are not (fermionic) supercharges here. Instead, we notice, taking the one-dimensional harmonic oscillator, that

$$H = \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega x^2\right)\sigma_3 = \frac{\hbar\omega}{2}\{A, A^\dagger\}, \tag{35}$$

with

$$A = \begin{pmatrix} a & 0 \\ 0 & \alpha a^\dagger \end{pmatrix}, \quad A^\dagger = \begin{pmatrix} a^\dagger & 0 \\ 0 & \beta a \end{pmatrix}, \quad \alpha\beta = -1 \tag{36}$$

being defined in terms of the usual annihilation and creation operators

$$a = \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{\mathrm{d}}{\mathrm{d}x} + \frac{m\omega}{\hbar}x\right), \quad a^\dagger = \sqrt{\frac{\hbar}{2m\omega}}\left(-\frac{\mathrm{d}}{\mathrm{d}x} + \frac{m\omega}{\hbar}x\right). \tag{37}$$

The relation of the Heisenberg algebra

$$[A, A^\dagger] = I \tag{38}$$

obviously holds true.

We immediately see that the operators (36) are not adjoint to each other, with respect to the usual scalar product.

To see more clearly what is behind this, let us go to the following Section.

4. A unified approach from both perspectives

We claim that reversing time has the same consequences, at least for the Hamiltonian, its eigenvalues and its eigenstates, as rotating spatial coordinates.

To enlighten this statement, we use the method of complex coordinate rotation first introduced with a real exponential (related to the dilatation group [21, 22]) and then extended to a complex exponential (for a review, see [23]) acting on the spatial coordinates:

$$x \mapsto x(\theta) = \mathrm{e}^{\mathrm{i}\theta}x. \tag{39}$$

This change of variables has been introduced in a different context than the one considered here i.e. the study of quasi-bound resonance states having a complex spectrum.

Nevertheless, we use this new coordinate system here to define generalized annihilation and creation operators through

$$a(\theta) \equiv \sqrt{\frac{\hbar}{2m\omega}}\left(\mathrm{e}^{-\mathrm{i}\theta}\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{e}^{\mathrm{i}\theta}\frac{m\omega}{\hbar}x\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{\mathrm{i}}{\hbar}p(\theta) + \frac{m\omega}{\hbar}x(\theta)\right), \tag{40}$$

$$a^\dagger(\theta) \equiv \sqrt{\frac{\hbar}{2m\omega}}\left(-\mathrm{e}^{-\mathrm{i}\theta}\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{e}^{\mathrm{i}\theta}\frac{m\omega}{\hbar}x\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(-\frac{\mathrm{i}}{\hbar}p(\theta) + \frac{m\omega}{\hbar}x(\theta)\right). \tag{41}$$

It is straightforward to convince ourselves that

$$[a(\theta), a^\dagger(\theta)] = 1, \tag{42}$$

as well as

$$\frac{\hbar\omega}{2}\left\{a(\theta), a^\dagger(\theta)\right\} = H(\theta) = -\mathrm{e}^{-2\mathrm{i}\theta}\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}\mathrm{e}^{2\mathrm{i}\theta}m\omega^2x^2. \tag{43}$$

It is then clear that the positive-energy Hamiltonian corresponds to $\theta = 0$ while the negative-energy one is related to $\theta = \frac{\pi}{2}$.

Solving

$$H(\theta)\phi = E\phi, \tag{44}$$

we are led to

$$E = -\hbar\omega\epsilon\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots \tag{45}$$

and the usual eigenstates (29). Here ϵ is defined according to

$$\begin{cases} \epsilon = -1 & \text{if } \theta = 0, \\ \epsilon = 1 & \text{if } \theta = \dfrac{\pi}{2}. \end{cases} \tag{46}$$

We thus recover the results (29)–(30) of the real (fourth-order) equation.

As the complex rotation method has no impact on the eigenvectors for the oscillator potential, we can introduce a new inner product whose only change is related to the transformation of the spatial coordinate

$$\langle\psi|\phi\rangle_\theta \equiv \mathrm{e}^{-\mathrm{i}\theta}\int \psi^*(x)\phi(x)\,\mathrm{d}x. \tag{47}$$

When positive energies are concerned ($\theta = 0$), we recover the usual Hermitian inner product while it becomes skew-Hermitian for negative energies ($\theta = \frac{\pi}{2}$). Skew-Hermiticity is actually what characterizes the negative-energies annihilation and creation operators since

$$a\left(\frac{\pi}{2}\right) = \sqrt{\frac{1}{2m\omega\hbar}}\,(p + \mathrm{i}m\omega x)\,, \quad a^\dagger\left(\frac{\pi}{2}\right) = \sqrt{\frac{1}{2m\omega\hbar}}\,(-p + \mathrm{i}m\omega x)\,, \tag{48}$$

and

$$p\left(\frac{\pi}{2}\right) = -\frac{\mathrm{d}}{\mathrm{d}x}, \quad x\left(\frac{\pi}{2}\right) = \mathrm{i}x. \tag{49}$$

Note that the presence of the phase factor in this new inner product does not change the probabilistic interpretation of quantum mechanics since transition probabilities are given par the product of the inner product by its complex conjugate.

We can also come back to the Ehrenfest theorem by mentioning that the mean values of the position and momentum operators now lead to

$$\langle x(\theta)\rangle_\theta = \mathrm{e}^{-\mathrm{i}\theta}\mathrm{e}^{\mathrm{i}\theta}\int \psi^* x\psi\,\mathrm{d}x = \langle x\rangle, \tag{50}$$

$$\langle p(\theta)\rangle_\theta = \mathrm{e}^{-\mathrm{i}\theta}\mathrm{e}^{-\mathrm{i}\theta}\int \psi^* p\psi \,\mathrm{d}x = -\langle p\rangle \quad \text{if} \quad \theta = \frac{\pi}{2}. \tag{51}$$

As a consequence, this new inner product allows us to find, in the unitary context, the sign change of the mean value of p, typical of the anti-unitary context.

Notice also that the idea of a new scalar product is not new. It has already been evoked in [24] (where we can find a mixed scalar product, the usual scalar product for the angular part of the Schrödinger equation and the scalar product without complex conjugation for the radial part) and [25] (in which a scalar product based on a time inversion only is introduced).

5. Conclusion

We have highlighted the arguments that allow us to affirm that the choice of anti-unitarity for time inversion is not as obvious as it seems at first sight...

Let us resume the different characteristics in a summary table (see Table 1).

anti-unitary T	unitary T
$\mathrm{i} \mapsto -\mathrm{i}$	$\mathrm{i} \mapsto i$
$\vec{p} \mapsto -\vec{p}$	$\vec{p} \mapsto \vec{p}$
$E \geq 0$	$\begin{cases} E \geq 0 \ (\theta = 0) \\ E \leq 0 \ (\theta = \frac{\pi}{2}) \end{cases}$

Table 1: The different features of anti-unitary T as well as unitary T.

In both cases, the fundamental relations and equations of non-relativistic quantum mechanics remain invariant.

The two versions, unitary and anti-unitary, are coherent, from a theoretical point of view. What will really decide in favor of one or the other option is the confirmed or denied existence of negative mass particles. Experiments such as those conducted in [26] will be crucial in this sense.

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Declaration of interests

☒The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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