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Time Reversal in Classical and Quantum Mechanics*

J. M. Domingos

Departamento de Física, Universidade de Coimbra, Coimbra, Portugal

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A review of Wigner's time reversal is presented and some important aspects are emphasized. The subject is introduced via classical mechanics. Nonphysical statements as "time running backwards" are avoided. Comments are made on the roles of time and of the operator $i\hbar(\partial/\partial t)$ in quantum mechanics. The role of symmetries and conservation laws and some properties of the time-reversed states are discussed.

1. TIME REVERSAL IN CLASSICAL MECHANICS

To illustrate the principles involved in time reversal, let us consider a simple problem in classical mechanics. Suppose a particle is moving along a trajectory (Figure 1) in a conservative field of force. The equation of motion is

$$m\frac{d^2\mathbf{r}}{dt^2} = -\nabla V \tag{1.1}$$

Let $\mathbf{r}_\text{I}(0)$ and $\mathbf{p}_\text{I}(0)$ be the position and momentum of the particle at the time $t = 0$. At this instant let us start the motion of an identical particle with position and momentum given by $\mathbf{r}_\text{II}(0) = \mathbf{r}_\text{I}(0)$ and $\mathbf{p}_\text{II}(0) = -\mathbf{p}_\text{I}(0)$. If the second particle retraces the trajectory, arriving at a later time $t = t_2$ to the position of the first particle at $t = -t_2$ with opposite momentum, we say that the equation of motion underlying the process is invariant under time reversal. That is, if the equations of motion allow $\mathbf{r}(t)$ as a possible trajectory for the particle, then $\mathbf{r}(-t)$ is also allowed.

We could instead speak of reversal of motion since it is realized with the time developing normally but reversing the momentum. Speaking about time running backwards could arise objections with respect to reversing the flow of time in an actual experiment. To understand time reversal one does

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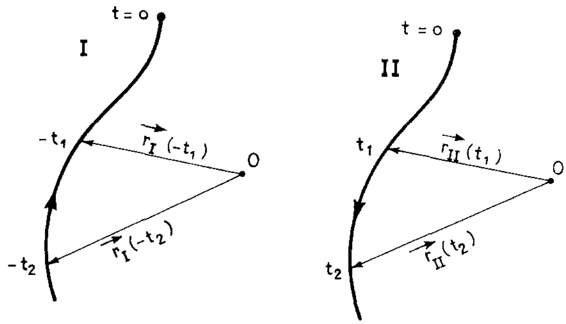

Fig. 1. Two classical trajectories I and II that correspond by time reversal. The two trajectories coincide but are shown separated for clarity.

not need to think in terms of time flowing backwards or in such refinements as the motion of the hands of the clock being reversed. The process could be illustrated by a film which when run backwards shows a motion compatible with the equations of motion, that is, as physically possible as the original. The improbability of the reversed motion does not worry us. It is enough that the process is, in principle, a possible one. Mathematically, once we know $\mathbf{r}_{\mathrm{I}}(t)$ we can express this correspondence by

$$\mathbf{r}_{\mathrm{II}}(t) = \mathbf{r}_{\mathrm{I}}(-t)$$

Considering the velocities we may write

$$\mathbf{v}_{\mathrm{I}}(t) = \left(\frac{d\mathbf{r}_{\mathrm{I}}(t)}{dt}\right)_t$$

$$\begin{aligned}\mathbf{v}_{\mathrm{II}}(t) &= \lim_{\Delta t\to 0} \frac{\mathbf{r}_{\mathrm{II}}(t+\Delta t) - \mathbf{r}_{\mathrm{II}}(t)}{\Delta t} \\ &= \lim_{\Delta t\to 0} \frac{\mathbf{r}_{\mathrm{I}}(-t-\Delta t) - \mathbf{r}_{\mathrm{I}}(-t)}{\Delta t} = -\left(\frac{d\mathbf{r}_{\mathrm{I}}(t)}{dt}\right)_{-t} = -\mathbf{v}_{\mathrm{I}}(-t)\end{aligned}$$

So

$$\mathbf{p}_{\mathrm{II}}(t) = -\mathbf{p}_{\mathrm{I}}(-t)$$

We can say that the time-reversed state of the particle is defined by

$$\mathbf{r}_{\mathrm{II}}(t) = \mathbf{r}_{\mathrm{I}}(-t)$$
$$\mathbf{p}_{\mathrm{II}}(t) = -\mathbf{p}_{\mathrm{I}}(-t)$$

Of course resulting from the transformations of $\mathbf{r}$ and $\mathbf{p}$ the angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ changes sign.

In general, for a system described by the generalized coordinates q_{I} and generalized momenta p_{I}, assuming that the Hamiltonian $H_{\mathrm{I}}(q_{\mathrm{I}}, p_{\mathrm{I}})$ does not depend explicitly on time, we may write the equations of motion

$$\begin{aligned} \frac{dq_{\mathrm{I}}}{dt} &= \frac{\partial H_{\mathrm{I}}(q_{\mathrm{I}}, p_{\mathrm{I}})}{\partial p_{\mathrm{I}}} \\ \frac{dp_{\mathrm{I}}}{dt} &= -\frac{\partial H_{\mathrm{I}}(q_{\mathrm{I}}, p_{\mathrm{I}})}{\partial q_{\mathrm{I}}} \end{aligned} \tag{1.2}$$

Let us suppose that another system II exists, so that for each solution $q_{\mathrm{I}}(t)$, $p_{\mathrm{I}}(t)$ of (1.2), a time-reversed solution

$$\begin{aligned} q_{\mathrm{II}}(t) &= q_{\mathrm{I}}(-t) \\ p_{\mathrm{II}}(t) &= -p_{\mathrm{I}}(-t) \end{aligned} \tag{1.3}$$

is allowed, satisfying

$$\begin{aligned} \left(\frac{dq_{\mathrm{II}}(t)}{dt}\right)_t &= -\left(\frac{dq_{\mathrm{I}}(t)}{dt}\right)_{-t} = -\frac{\partial H_{\mathrm{I}}(q_{\mathrm{I}}(-t), p_{\mathrm{I}}(-t))}{\partial p_{\mathrm{I}}(-t)} \\ &= \frac{\partial H_{\mathrm{I}}(q_{\mathrm{II}}(t), -p_{\mathrm{II}}(t))}{\partial p_{\mathrm{II}}(t)} = \frac{\partial H_{\mathrm{II}}(q_{\mathrm{II}}(t), p_{\mathrm{II}}(t))}{\partial p_{\mathrm{II}}(t)} \\ \left(\frac{dp_{\mathrm{II}}(t)}{dt}\right)_t &= \left(\frac{dp_{\mathrm{I}}(t)}{dt}\right)_{-t} = -\frac{\partial H_{\mathrm{I}}(q_{\mathrm{I}}(-t), p_{\mathrm{I}}(-t))}{\partial q_{\mathrm{I}}(-t)} \\ &= -\frac{\partial H_{\mathrm{I}}(q_{\mathrm{II}}(t), -p_{\mathrm{II}}(t))}{\partial q_{\mathrm{II}}(t)} = -\frac{\partial H_{\mathrm{II}}(q_{\mathrm{II}}(t), p_{\mathrm{II}}(t))}{\partial q_{\mathrm{II}}(t)} \end{aligned}$$

For this to be true for all the solutions $q_{\mathrm{I}}(t)$, $p_{\mathrm{I}}(t)$, the Hamiltonian of the system II should be obtained from the Hamiltonian of system I by changing the signs of the momenta. If we are considering the time development of *the same system* then the Hamiltonian must be invariant under this operation. This is what happens in many cases of physical interest, when for example it is quadratic in the momenta. We say that the equations of motion are invariant under time reversal. Quantitatively, we may say that the time reversal invariance in classical mechanics is a consequence of the invariance of the equations of motion under the transformation $t \to -t$. In this way $d/dt \to -d/dt$, $q \to q$, $\dot{q} \to -\dot{q}$, $p \to -p$, and $\dot{p} \to \dot{p}$, and if the Hamiltonian is left invariant by the transformation, Hamilton's equations are invariant.

Nevertheless there are very important classical systems evolving in the presence of external fields. Then the invariance holds or not according to the behavior of the external forces under time reversal. In particular, and referring to Fig. 1, the invariance holds if the external forces for $\mathbf{r}_{\mathrm{II}}$ at time t, are the same as the external forces for $\mathbf{r}_{\mathrm{I}}$ at time $-t$. A simple example where it is not so is the case of the frictional forces because these forces change sign in the reversed motion. Another simple example is the motion of a charged particle in a time-independent magnetic field. Due to the Lorentz force

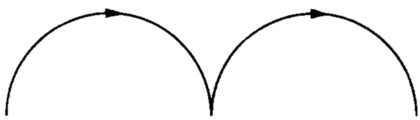

Fig. 2. Time reversal trajectories of a charged particle in a magnetic field. The field is assumed normal to the plane of the page.

changing sign with inversion of the velocity, time reversal invariance does not hold. The situation can be visualized in Figure 2.

The difficulty is obvious if we write, for example, the Hamiltonian describing a nonrelativistic particle in an electromagnetic field

$$H = \left\{\frac{1}{m}\left[\mathbf{p} - \frac{e}{c}\,\mathbf{A}(\mathbf{r}, t)\right]^2 + eA_0(\mathbf{r}, t)\right\} \tag{1.4}$$

where $\mathbf{A}$ is the vector potential and A_0 is the scalar potential.

$\mathbf{A}$ is itself created by charges in motion. If we incorporate these charges in our system, we change by time reversal the sign of $\mathbf{A}$, and therefore the magnetic field, but the electric field generated by the charges, remains the same.

The scheme fails if we are interested in studying the motion of a charge in a fixed external field.

What we mean is that, if the charged particle is moving in an external field, to have a time reversal invariant Hamiltonian we have to accept a more general definition of the time-reversed state:

$$\begin{aligned} \mathbf{r}_{\mathrm{II}}(t) &= \mathbf{r}_{\mathrm{I}}(-t) \\ \mathbf{p}_{\mathrm{II}}(t) &= -\mathbf{p}_{\mathrm{I}}(-t) \\ \mathbf{A}_{\mathrm{II}}(\mathbf{r}, t) &= -\mathbf{A}_{\mathrm{I}}(\mathbf{r}, -t) \\ A_{0\mathrm{II}}(\mathbf{r}, t) &= A_{0\mathrm{I}}(\mathbf{r}, -t) \end{aligned}$$

Maxwell's equations are, in particular, unchanged under time reversal.

2. THE ROLE OF TIME IN QUANTUM MECHANICS

The Schrödinger formulation of quantum mechanics is based on a description where the state vector moves about in Hilbert space, as time develops.

Assuming that no measurements are made, an isolated system evolves in a uniquely predicted way. In the case of an isolated system the Hamiltonian is time independent and the time evolution operator

$$U(t) = \exp\left\{-\frac{i}{\hbar}Ht\right\} \tag{2.1}$$

where t is a parameter which may take any value from $-\infty$ to $+\infty$, has the job of "driving" $|\psi(t)\rangle$ in Hilbert space. This transformation operator is similar in form to the operator $\exp\{-(i/\hbar)pa\}$, where a is a real parameter. This operator, when acting on the ket $|x'\rangle$, corresponds to the eigenvalue $x' + a$ which may be any value from $-\infty$ to $+\infty$. That is, the spectrum of x is continuous and extends from $-\infty$ to $+\infty$. Analogously the unitary operator $\exp\{(i/\hbar)xb\}$ corresponds, when acting on the ket $|p'\rangle$, to eigenvalues of p which may have any value from $-\infty$ to $+\infty$. We could ask (Pauli, 1958) at this stage if there is a time operator T, generator of energy displacements, such that $\exp\{(i/\hbar)Te\}$, with e an energy parameter, when applied to a ket $|E\rangle$ would correspond to an eigenvalue $E + e$ of the Hamiltonian H. Similarly, to the x-p problem, if such a time operator T existed, corresponding to a commutation relation $[T, H] = i\hbar$, a continuous spectrum of energy would result from $-\infty$ to $+\infty$. The occurrence of discrete eigenvalues of H, which imply that the spectrum of H is bounded from below, $E > E_{\min}$, invalidates the hypothesis that such an operator T exists. So energy and time appear in quantum theory on a completely different footing: the energy is a dynamical variable but the time is a parameter and does not correspond to the eigenvalue of an Hermitian operator. In particular the time-energy uncertainty relation has to be put in a different way from the coordinate-momentum uncertainty relation.

In a nonisolated system, H is time dependent and $U(t)$ has not the simple form of (2.1), but the time evolution of the state vector $|\psi(t)\rangle$ is still given by the Schrödinger equation

$$H(t)|\psi(t)\rangle = i\hbar \frac{\partial|\psi(t)\rangle}{\partial t} \tag{2.2}$$

Some care is necessary when writing an expression like

$$H = i\hbar \frac{\partial}{\partial t} \tag{2.3}$$

The Hamiltonian is an operator whose form is determined by the properties of the system and is a function of operators like coordinate and momentum. The Hamiltonian H is an operator in Hilbert space, but $i\hbar(\partial/\partial t)$, which acts on the family $|\psi(t)\rangle$ of a continuous parameter t, is not an operator in Hilbert space. What is involved in equation (2.2) is to find a parametrization of the family $|\psi(t)\rangle$ in Hilbert space so that H acting on the state vector $|\psi(t)\rangle$ gives the same result as $i\hbar(\partial/\partial t)$ acting on $|\psi(t)\rangle$. Let us see this point with a little more detail. An operator A in Hilbert space is determined, only, by its effect on the basis vectors $|\varphi_\alpha\rangle$

$$A|\varphi_\alpha\rangle = \sum_\beta |\varphi_\beta\rangle a_{\beta\alpha}$$

Writing the state vector $|\psi(t)\rangle$ as

$$|\psi(t)\rangle = \sum_\beta c_\beta(t)|\varphi_\beta\rangle$$

where $c_\beta(t)$ stands for the amplitude to be in the base state $|\varphi_\beta\rangle$ at the time t, Schrödinger equation tells us that

$$i\hbar \frac{dc_\alpha(t)}{dt} = \sum_\beta H_{\alpha\beta} c_\beta(t) \tag{2.4}$$

with

$$H_{\alpha\beta} = \langle\varphi_\alpha|H|\varphi_\beta\rangle$$

3. TIME REVERSAL IN QUANTUM MECHANICS

We shall discuss the operation known as Wigner time reversal, first introduced by Wigner in 1932.

To start with, let us suppose that $|\psi(t)\rangle$ is a solution of the Schrödinger equation

$$H|\psi(t)\rangle = i\hbar \frac{\partial|\psi(t)\rangle}{\partial t} \tag{3.1}$$

with H a time-independent Hamiltonian.

If we replace t by $-t$ this equation becomes

$$H|\psi(-t)\rangle = -i\hbar \frac{\partial|\psi(-t)\rangle}{\partial t}$$

showing that the Schrödinger equation is not invariant under the transformation $t \to -t$.

For comparison, let us consider the heat-conduction equation, which also involves a first-order time derivative,

$$\frac{\partial T}{\partial t} = k\nabla^2 T \tag{3.2}$$

where k is the thermal diffusivity and T the temperature. This equation reflects an asymmetry in time in the process of, say, the distribution of energy when two pieces of metal at different temperatures are placed in contact with each other. But in spite of both equations (3.1) and (3.2) being of first order in time, the presence of i in the Schrödinger equation not only allows periodic solutions, but also enables the original form to be restored by taking its complex conjugate. In fact, if H is real,

$$H|\psi(-t)\rangle^* = i\hbar \frac{\partial|\psi(-t)\rangle^*}{\partial t}$$

and $|\psi(-t)\rangle^*$ satisfies the same Schrödinger equation as $|\psi(t)\rangle$.

The invariance would be assured if besides replacing t by $-t$, we consider the effect of the operator complex conjugation to reproduce the form of the Schrödinger equation. That is, even if $|\psi(-t)\rangle$ is not a solution it is possible to find an antilinear operator that transforms $|\psi(-t)\rangle$ into the time-reversed solution $|\psi_R(t)\rangle$ of the Schrödinger equation.

As required, this transformation ensures that if the system is in a time-reversed state $|\psi_R(t)\rangle$, the probability of finding it in a state $|\phi_R(t)\rangle$ is equal to the probability of finding it, at the time $-t$, in the state $|\phi(t)\rangle$ when the system is known to be the original state $|\psi(t)\rangle$. In fact, as

$$\langle\phi_R(t)|\psi_R(t)\rangle = \langle\phi(-t)|\psi(-t)\rangle^* \tag{3.3}$$

we have

$$|\langle\phi_R(t)|\psi_R(t)\rangle|^2 = |\langle\phi(-t)|\psi(-t)\rangle|^2$$

Without alteration in the result, and for reasons that will shortly be clarified, we shall include a unitary operator U in the definition of the time reversal operator

$$|\psi_R(t)\rangle = U|\psi(-t)\rangle^* = UK|\psi(-t)\rangle = \mathscr{T}|\psi(-t)\rangle \tag{3.4}$$

with K the complex conjugation operator. As we shall see, the choice $\mathscr{T} = K$ is only correct in a particular representation, $\mathscr{T} = UK$ being a more general time reversal operator.

The operator $\mathscr{T} = UK$ is antiunitary, i.e., is antilinear and preserves the norm

$$(\langle\psi|\mathscr{T}^\dagger)(\mathscr{T}|\psi\rangle) = \langle\psi|\psi\rangle \tag{3.5}$$

The effect of the operator K depends on the representation used. Considering the particular basis vectors corresponding to a representation, the state vector is represented by its coefficients. By definition $|\psi(t)\rangle^*$ is the vector obtained taking, on the same basis, the complex conjugate of these coefficients. If

$$|\psi\rangle = \sum_i |a_i\rangle\langle a_i|\psi\rangle$$

then

$$|\psi\rangle^* = \sum_i |a_i\rangle\langle a_i|\psi\rangle^*$$

We also define the complex conjugate operator as

$$O^* = \sum_{i,j} |a_i\rangle\langle a_i|O|a_j\rangle^*\langle a_j|$$

Since the operation of complex conjugation carried out twice is equivalent to the identity operation, $K^2 = I$ and therefore $K = K^{-1}$, we may write $\mathscr{T}^{-1} = KU^\dagger$.

Summarizing, and in more general terms, let $|\psi(t)\rangle$ be a solution of the Schrödinger equation

$$H(t)|\psi(t)\rangle = i\hbar \frac{\partial|\psi(t)\rangle}{\partial t}$$

Considering the equation

$$H^*(-t)|\psi(-t)\rangle^* = i\hbar \frac{\partial|\psi(-t)\rangle^*}{\partial t}$$

if there is a unitary operator U such that

$$\mathscr{T} H(-t)\mathscr{T}^{-1} = UH^*(-t)U^\dagger = H(t) \tag{3.6}$$

we may write

$$UH^*(-t)U^\dagger U|\psi(-t)\rangle^* = i\hbar \frac{\partial U|\psi(-t)\rangle^*}{\partial t}$$

in the form

$$H(t)|\psi_R(t)\rangle = i\hbar \frac{\partial|\psi_R(t)\rangle}{\partial t}$$

If $|\psi(t)\rangle$ is a solution, $|\psi_R(t)\rangle = \mathscr{T}|\psi(-t)\rangle$ is a solution.

The unitary operator U depends on the nature of the Hamiltonian and like K depends on the representation used for the wave function, as we shall see in examples which will later be considered.

Now we shall consider for a single particle state the real expectation values of the coordinate and momentum operators. By analogy with the classical problem we would like the transformation properties of the operators $\mathbf{r}$ and $\mathbf{p}$, under time reversal, to be such that

$$\langle\psi(-t)|\mathbf{r}|\psi(-t)\rangle = \langle\psi_R(t)|\mathbf{r}|\psi_R(t)\rangle \tag{3.7}$$

$$\langle\psi(-t)|\mathbf{p}|\psi(-t)\rangle = -\langle\psi_R(t)|\mathbf{p}|\psi_R(t)\rangle \tag{3.8}$$

Remembering the classical definition of time-reversed states this is exactly what we should expect when comparing the expectation values for the state $|\psi_R(t)\rangle$ with the expectation values for the state $|\psi(t)\rangle$ at the time $-t$. We shall see next that the transformations

$$\mathscr{T}\mathbf{r}\mathscr{T}^{-1} = \mathbf{r}, \qquad \mathscr{T}\mathbf{p}\mathscr{T}^{-1} = -\mathbf{p} \tag{3.9}$$

satisfy the results (3.7) and (3.8). In fact,

$$\begin{aligned}\langle\psi(-t)|\mathbf{r}|\psi(-t)\rangle &= \langle\psi(-t)|(\mathscr{T}^{-1}\mathscr{T}\mathbf{r})|\psi(-t)\rangle \\ &= (\langle\psi(-t)|\mathscr{T}^{-1})\mathbf{r}(\mathscr{T}|\psi(-t)\rangle) = \langle\psi_R(t)|\mathbf{r}|\psi_R(t)\rangle\end{aligned}$$

and

$$\begin{aligned}\langle\psi(-t)|\mathbf{p}|\psi(-t)\rangle &= \langle\psi(-t)|(\mathscr{T}^{-1}\mathscr{T}\mathbf{p})|\psi(-t)\rangle \\ &= -(\langle\psi(-t)|\mathscr{T}^{-1})\mathbf{p}(\mathscr{T}|\psi(-t)\rangle) = -\langle\psi_R(t)|\mathbf{p}|\psi_R(t)\rangle\end{aligned}$$

The transformation properties (3.9) also preserve the commutation relation

$$[q_i, p_j] = i\hbar\delta_{ij}$$

In the same way the transformation properties for the orbital angular momentum

$$\mathscr{T} L_i \mathscr{T}^{-1} = -L_i$$

keep invariant commutation relations as

$$[L_x, y] = i\hbar z$$
$$[L_x, p_y] = i\hbar p_z$$
$$[L_x, L_y] = i\hbar L_z$$

Even if the spin has no classical analogous, its angular momentum properties suggest that it must transform like the orbital angular momentum

$$\mathscr{T} s_i \mathscr{T}^{-1} = -s_i$$

As the time is just a real parameter the time reversal operator does not act on t:

$$\mathscr{T} t \mathscr{T}^{-1} = t$$

We shall now discuss some relevant cases.

(a) The Hamiltonian describes a spinless particle.

Let us consider in the first place the coordinate representation.

We may write

$$\mathscr{T}\mathbf{r}\psi = U\mathbf{r}\psi^* = \mathbf{r}\mathscr{T}\psi = \mathbf{r}U\psi^*$$

and so U commutes with the operator of the coordinates.

In the coordinate representation $\mathbf{p} = -i\hbar\nabla$ and, as U is a linear operator,

$$\mathscr{T}(-i\hbar\nabla)\psi = i\hbar U\nabla\psi^* = i\hbar\nabla\mathscr{T}\psi = i\hbar\nabla U\psi^*$$

it follows that U commutes with $\mathbf{r}$ and ∇ and so it cannot be either a function of the coordinates or a differential operator of the coordinates. It follows that U has to be, in the coordinate representation, equivalent to the multiplication by a constant of modulus unity. The operator U is only determined up to a phase factor. In fact, since we can always multiply the wave function by a phase factor we can combine the effect of the operator U with a further phase factor. So we can choose $U = 1$ and write in the coordinate representation

$$\mathscr{T} = K$$

and

$$\psi_R(\mathbf{r}, t) = \psi^*(\mathbf{r}, -t)$$

and if H is not explicitly time dependent the condition $UH^*U^{-1} = H$ for a spin-independent Hamiltonian in the coordinate representation, is simply

$$H^* = H \qquad \text{(real)}$$

In the momentum representation $\mathbf{r} = i\hbar\nabla_p$ and $K\mathbf{p}K^{-1} = \mathbf{p}^* = \mathbf{p}$. We may note that we cannot say that $\mathbf{r}$ or $\mathbf{p}$ are real or imaginary without specifying the representation.

The time reversal operator in the momentum representation cannot be written simply as K. We should write

$$\mathscr{T} = U_p K$$

with the definition

$$U_p \mathbf{p} U_p^{-1} = -\mathbf{p}$$

Thus U_p is simply the operation of replacing every momentum $\mathbf{p}$ by $-\mathbf{p}$. So, we write

$$\psi_R(\mathbf{p}, t) = \psi^*(-\mathbf{p}, -t)$$

We obtain

$$\mathscr{T}\mathbf{r}\mathscr{T}^{-1} = U_p K(i\hbar\nabla_p)KU_p{}^\dagger = i\hbar\nabla_p = \mathbf{r}$$
$$\mathscr{T}\mathbf{p}\mathscr{T}^{-1} = U_p K\mathbf{p}KU_p{}^\dagger = -\mathbf{p}$$

and of course, the condition $UH^*U^{-1} = H$ is written

$$U_p H^* U_p^{-1} = H$$

If, for example, the Hamiltonian contains terms of interaction with an electromagnetic field, it is obvious that in the coordinate representation $U = U_A$ where

$$U_A \mathbf{A}(\mathbf{r}, -t)U_A^{-1} = -\mathbf{A}(\mathbf{r}, -t) \tag{3.10}$$

and in the momentum representation

$$U = U_p U_A$$

(b) The Hamiltonian describes a nonrelativistic spin-$\frac{1}{2}$ particle.

As we know the nonrelativistic spin-$\frac{1}{2}$ theory requires a two-component wave function, corresponding to the two degrees of freedom of the spin.

Using the coordinate representation we have only to determine U_σ in spin space. In accordance with previous considerations we may write

$$U_\sigma K\boldsymbol{\sigma}K^{-1}U_\sigma^{-1} = -\boldsymbol{\sigma}$$

and using the Pauli matrices in the usual representation

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.11}$$

the operator U_σ must satisfy

$$U_\sigma \sigma_x U_\sigma^\dagger = -\sigma_x$$
$$U_\sigma \sigma_y U_\sigma^\dagger = \sigma_y$$
$$U_\sigma \sigma_z U_\sigma^\dagger = -\sigma_z$$

and we may write $U_\sigma = e^{i\delta}\sigma_y$, with δ an arbitrary phase. A choice that makes U_σ real is

$$U_\sigma = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{3.12}$$

We may write in the $|\mathbf{r}, m_s\rangle$ basis

$$\mathscr{T} = i\sigma_y K \tag{3.13}$$

Incidentally, as we shall see, this is also the form of the time reversal operator in Dirac theory.

If H does not depend explicitly on time, it is invariant under time reversal provided that

$$\sigma_y H^* \sigma_y = H \tag{3.14}$$

We may note that once $s_y = (\hbar/2)\sigma_y$ we may write U_σ as a rotation by $-\pi$ about the y axis in spin space. In fact

$$R_y^{-1}(\pi) = \exp\left\{\frac{i}{\hbar}\pi s_y\right\} = \exp\left\{i\frac{\pi}{2}\sigma_y\right\} = I\cos\frac{\pi}{2} + i\sigma_y \sin\frac{\pi}{2} = i\sigma_y = U_\sigma$$

For a system of N spin-$\frac{1}{2}$ particles

$$\mathscr{T} = i^N \prod_{n=1}^{N} \sigma_y(n) K \tag{3.15}$$

(c) The Hamiltonian describes a relativistic spin-$\frac{1}{2}$ particle.

For a particle in an electromagnetic field $(A_0, \mathbf{A})$ we can write Dirac's equation in Hamiltonian form:

$$H\psi(\mathbf{r}, t) = i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = \left[c\boldsymbol{\alpha}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r}, t)\right) + \beta m_0 c^2 + eA_0\right]\psi(\mathbf{r}, t) \tag{3.16}$$

where the wave function ψ has four components (it is not a four-vector) and α^k and β are 4×4 Hermitian matrices acting on spin space and satisfying

$$\alpha^k\alpha^l + \alpha^l\alpha^k = 2\delta^{kl} \qquad (k, l = 1, 2, 3)$$
$$\alpha^k\beta + \beta\alpha^k = 0$$
$$(\alpha^k)^2 = \beta^2 = I$$

With the help of Pauli's matrices σ_k and the 2×2 unit matrix I, they are, written in Dirac's representation,

$$\alpha^k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{3.17}$$

The time reversal operator has the form $\mathscr{T} = UK$, where U contains, besides the operator U_A which transforms $\mathbf{A}(\mathbf{r}, -t)$, an operator U_D, acting only on the matrices α^k and β, needed to bring the transformed Dirac's equation

$$i\hbar \frac{\partial U_D\psi^*(\mathbf{r}, -t)}{\partial t}$$

$$= \left\{-cU_D\boldsymbol{\alpha}^* U_D^{-1}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r}, -t)\right) + U_D\beta^* U_D^{-1} m_0c^2 + eA_0\right\} U_D\psi^*(\mathbf{r}, -t)$$

to the original form. So, it is straightforward that U_D should give

$$U_D\alpha^{k*}U_D^{-1} = -\alpha^k$$

$$U_D\beta^*U_D^{-1} = \beta$$

The matrix U_D which gives the required transformation properties may be written, up to a phase,

$$U_D = \alpha^3\alpha^1 = i\hat{\sigma}_2 \tag{3.18}$$

where $\hat{\sigma}_2$ is the 4×4 matrix

$$\hat{\sigma}_2 = \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix} \tag{3.19}$$

So, we obtain a formally similar result to the nonrelativistic case.

We could have considered Dirac's equation in covariant form

$$\left[\gamma^\mu\left(i\hbar\frac{\partial}{\partial x^\mu} - \frac{e}{c}A_\mu\right) - m_0c\right]\psi(x) = 0 \tag{3.20}$$

where

$$\gamma^k = \beta\alpha^k$$

and

$$\gamma^0 = \beta$$

In Dirac's representation

$$\gamma^k = \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0 \end{pmatrix}, \qquad \gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{3.21}$$

With this choice γ^0 is Hermitian but the γ^k are antiHermitian matrices. The anticommutator of γ^μ and γ^ν satisfies

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$$

with $g^{\mu\nu}$ the metric tensor

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Considering the transformed equation

$$\Big\{ U_D \gamma^{0*} U_D^{-1} \left[i\hbar \frac{\partial}{\partial x^0} - \frac{e}{c} A_0(-x^0, x^k) \right] + \sum_{k=1}^{3} U_D(-\gamma^{k*}) U_D^{-1} \left[i\hbar \frac{\partial}{\partial x^k} - \frac{e}{c} A_k(-x^0, x^k) \right] - m_0 c \Big\} U_D \psi^*(-x^0, x^k) = 0$$

the matrix U_D which recovers the original form may be written, up to a phase,

$$U_D = \gamma^1 \gamma^3$$

and we may write besides the operator U_A

$$\mathscr{T} = \gamma^1 \gamma^3 K = i\hat{\sigma}_2 K \tag{3.22}$$

4. THE ASSOCIATION OF SYMMETRY OPERATIONS WITH CONSERVATION LAWS AND THE TIME REVERSAL OPERATION

If a physical system possesses a complete set of commuting observables, $A, B, \ldots, L$, the corresponding eigenvalues completely determine a state $|a, b, \ldots, 1\rangle$, which is unique up to a phase. Allowing each of the eigenvalues to vary over its spectrum we obtain an orthonormal basis. When speaking of a "state" we shall mean a state $|\psi\rangle$ which can be identified by the coefficients of the linear combination of the basis vectors, so that the phase relations between those components are known.

When we can assign to a system a definite state (often called a pure state), the set of vectors $e^{i\delta}|\psi\rangle$ is called a ray and all vectors belonging to a ray represent the same physical state.

The transition probability $|\langle\phi|\psi\rangle|^2$ represents the probability of the system known to be in the state $|\psi\rangle$ behaving as if it were in state $|\phi\rangle$.

A symmetry operation (sometimes referred to as invariance principle) applied to a state is a one-to-one correspondence which assigns to every physical state $|\psi\rangle$ another state $|\psi'\rangle$ in a way that the physical properties (transition probabilities and expectation values) are preserved.

Considering a symmetry operator T

$$|\psi'\rangle = T|\psi\rangle$$

we have, if it is either unitary or antiunita y,

$$TT^{\dagger} = T^{\dagger}T = I$$

Clearly, both unitary and antiunitary operators satisfy

$$|\langle\phi'|\psi'\rangle|^2 = |\langle\phi|\psi\rangle|^2 \tag{4.1}$$

Considering an arbitrary linear operator O (Hermitian or not), since the expectation values are preserved, we have for a *unitary* operator U

$$\langle\psi|O|\psi\rangle = \langle\psi'|O'|\psi'\rangle = \langle\psi|U^{\dagger}O'U|\psi\rangle$$

with the transformed operator

$$O' = UOU^{\dagger} \tag{4.2}$$

For an *antiunitary* operator $\mathscr{T}$

$$\langle\psi|O|\psi\rangle = \langle\psi'|O'|\psi'\rangle = (\langle\psi|\mathscr{T}^{\dagger})O'(\mathscr{T}|\psi\rangle) = \langle\psi|\mathscr{T}^{\dagger}O'\mathscr{T}|\psi\rangle^* = \langle\psi|O^{\dagger}|\psi\rangle^*$$

with the transformed operator

$$O' = \mathscr{T}O^{\dagger}\mathscr{T}^{\dagger} \tag{4.3}$$

In any case if

$$O' = O$$

we say that the operator is invariant under the symmetry transformation.

As we know, a unitary operator that corresponds to a continuous transformation can be written as

$$U = e^{i\epsilon A} \tag{4.4}$$

where ϵ is a parameter that varies continuously and A is a Hermitian operator called the generator. With a continuous transformation we can, from the identity operation, make a finite transformation out of infinitesimal ones. By making ϵ infinitesimal and keeping terms up to the order ϵ we may write

$$U = I + i\epsilon A + O(\epsilon^2)$$

If the Hamiltonian is invariant under the transformation, we have

$$UHU^{\dagger} = H = H + i\epsilon[A, H]$$

and the condition is equivalent to

$$[A, H] = 0$$

As the rate of change of the expectation value of an observable is determined by the commutator $[A, H]$ we see that if the Hamiltonian is invariant under a symmetry transformation the expectation value of the corresponding generator is a conserved quantity. For example, associated with the momentum, energy, and angular momentum operators we have translational invariance in space and time and rotational invariance, resulting in the consequent conservation principles.

Besides the continuous transformation operators we shall consider now discrete symmetry operators, by which we mean symmetry operators which if applied twice to a physical system leave the system unchanged. To this category belong, for example, parity and time reversal. It may happen that the symmetry operator is Hermitian and unitary, as the parity operator, and in this case if

$$PHP^{\dagger} = H, \qquad [P, H] = 0$$

the operator leads by itself to a symmetry operation and to a conservation principle. But the time reversal operator $\mathscr{T}$ is antilinear and so there is no corresponding conservation principle. In fact, since $\mathscr{T}$ is antilinear it cannot be a Hermitian operator. It does not make sense to associate with $\mathscr{T}$ either definite eigenvalues or definite eigenstates. Let us assume that the state vector $|\psi\rangle$ was an eigenstate of $\mathscr{T}$:

$$\mathscr{T}|\psi\rangle = a|\psi\rangle$$

By multiplication of $|\psi\rangle$ by a phase factor $e^{i\delta}$ we obtain the same physical state, but applying $\mathscr{T}$ we obtain

$$\mathscr{T}(e^{i\delta}|\psi\rangle) = e^{-i\delta}\mathscr{T}|\psi\rangle = e^{-i2\delta}a(e^{i\delta}|\psi\rangle)$$

So, resulting from its antilinearity, $\mathscr{T}$ cannot have a definite eigenvalue. Therefore $\mathscr{T}$ cannot be an observable and $\mathscr{T}$ does not give rise to a quantum number as parity does.

However, the operator $\mathscr{T}^2$ is a linear operator.

If the operator $\mathscr{T}$ is carried out twice in any state, we should obtain, independently of a change in phase, the same state apart from a factor

$$\mathscr{T}^2|\psi\rangle = c|\psi\rangle \tag{4.5}$$

That is, all states are eigenstates of $\mathscr{T}^2$, which is therefore a constant multiple of the unit operator and commutes with all observables

$$\mathscr{T}^2 = cI$$

or

$$\mathscr{T} = c\mathscr{T}^{\dagger}$$

and so

$$\mathscr{T}^{\dagger} = c^*\mathscr{T}$$

which substituted in the previous equation gives $|c|^2 = 1$, and so c is just a phase factor.

As

$$\mathscr{T}^\dagger\mathscr{T} = I$$

we may write

$$\mathscr{T}^2 = c\mathscr{T}^\dagger\mathscr{T}$$

and acting with $\mathscr{T}$ from the left and $\mathscr{T}^\dagger$ from the right, we obtain $\mathscr{T}c\mathscr{T}^\dagger = c$, that is, $c^* = c$ and therefore $c = \pm 1$. So we may write

$$\mathscr{T}^2 = \pm I \tag{4.6}$$

This result does not depend either on phase conventions or on the representation.

Seeing that $\mathscr{T}$ is a symmetry operator of the Hamiltonian

$$\mathscr{T}H\mathscr{T}^\dagger = H$$

we can expect the occurrence of additional degeneracies in the energy eigenstates. If the Hamiltonian of the N spin-$\frac{1}{2}$ particles is invariant under time reversal and if $|\psi_n\rangle$ is an energy eigenstate, from

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

we have

$$\mathscr{T}H|\psi_n\rangle = E_n\mathscr{T}|\psi_n\rangle$$

or

$$H\mathscr{T}|\psi_n\rangle = E_n\mathscr{T}|\psi_n\rangle$$

So if $|\psi_n\rangle$ is an eigenstate of a time reversal invariant Hamiltonian with energy E_n, the state $\mathscr{T}|\psi_n\rangle$ is also an eigenstate of H with energy E_n.

If $\mathscr{T}^2 = -I$ we can say that the state $\mathscr{T}|\psi_n\rangle$ is essentially different from $|\psi_n\rangle$, implying a twofold degeneracy known as Kramer's degeneracy, but if $\mathscr{T}^2 = +I$ we cannot say, without explicit details of the state, if they are the same state (up to a phase) or not. To examine this point we could go back to (3.15) and write for a system of N spin-$\frac{1}{2}$ particles

$$\mathscr{T}^2 = (-)^N I$$

The $+$ sign applies to an even number N of spin-$\frac{1}{2}$ particles and the $-$ sign to N odd. But we could look at the problem considering, to be more precise, eigenstates $|\alpha EJM\rangle$ of a time reversal invariant Hamiltonian, which are simultaneous eigenstates of J^2 and J_z, with α representing the set of all the other quantum numbers not related with the rotational properties of the state.

Resulting from (3.15) it is possible to choose the phases of the many-particle state so that

$$\mathscr{T}|\alpha EJM\rangle = (-)^{J+M}|\alpha EJ - M\rangle$$

It follows that

$$\mathscr{T}^2|\alpha EJM\rangle = (-)^{2J}|\alpha EJM\rangle$$

With J integer we have $\mathscr{T}^2 = +I$ and we cannot say, without further specification, if $\mathscr{T}|\alpha EJM\rangle$ is, up to a phase, the same state as $|\alpha EJM\rangle$ or if it is a different state.

With J half-odd integer we have $\mathscr{T}^2 = -I$ and then $\mathscr{T}|\alpha EJM\rangle$ is always different from $|\alpha EJM\rangle$ (they are linearly independent), the stationary states are pairwise degenerate, and it can be shown that they are orthogonal. In fact,

$$(\langle\psi|\mathscr{T}^\dagger)|\psi\rangle = (\langle\psi|\mathscr{T})|\psi\rangle = (\langle\psi|\mathscr{T}^\dagger)\mathscr{T}^2|\psi\rangle = -(\langle\psi|\mathscr{T}^\dagger)|\psi\rangle = 0$$

Since $\mathscr{T}^2$ commutes with all observables

$$\mathscr{T}^2 A \mathscr{T}^{-2} = A$$

and so the matrix elements of all observables connecting states with J integer (J_i) and J half-odd integer (J_{hi}) vanish. In fact

$$\langle J_i|A|J_{hi}\rangle = \langle J_i|\mathscr{T}^{-2}A\mathscr{T}^2|J_{hi}\rangle = -\langle J_i|A|J_{hi}\rangle = 0$$

So no transitions between any pair of such states, belonging to different eigenvalues of $\mathscr{T}^2$, can occur and so no physical measurements can determine their relative phase. There is said to be a superselection rule between the two sets of states, forbidding the comparison of their relative phases.

A superselection rule results from a conserved observable which commutes with all observables, which is equivalent to saying that all physical states are sharp eigenstates of the conserved observable. So we cannot observe in nature a physical state superposition of states corresponding to different values of $\mathscr{T}^2$.

We can say that the operator which is in the origin of the superselection rule separates the Hilbert space of physical state vectors into subspaces which are incoherent, and a linear combination of states of these subspaces, with known relative phases, is not physically realizable.

The ordinary selection rules, related to a physical process between subspaces belonging to different eigenvalues of a conserved observable, differ from the superselection rules because then not all physical states are eigenstates of the conserved observable.

The existence of symmetries, which must be checked experimentally, is a powerful tool to derive predictions, to find quantum numbers, to establish selection rules and useful phase relationships, and to restrict possible terms in the Hamiltonian, even if the dynamical theory involved is not fully known.

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