Time reversal of pseudo-spin $1/2$ degrees of freedom

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Abstract
We show that pseudo-spin $1/2$ degrees of freedom can be categorized in two types according to their behavior under time reversal. One type exhibits the properties of ordinary spin whose three Cartesian components are all odd under time reversal. For the second type, only one of the components is odd while the other two are even. We discuss several physical examples for this second type of pseudo-spin and highlight observable consequences that can be used to distinguish it from ordinary spin.

Keywords: foundations of quantum mechanics, reversal of motion, dynamical symmetry

1. Introduction
The behavior under time reversal (TR; also denoted reversal of motion) is one of the most fundamental characteristics of a quantum system [1, 2]. It determines, e.g., level degeneracies [3] and the statistics of energy-level spacings [4] in closed systems, electric transport in phase-coherent quantum circuits [5, 6], and the possible channels for pairing of electrons to form a superconducting Cooper-pair condensate [7]. Formally, the TR operation can be represented by an anti-unitary operator $\hat{\theta}$ that is, however, specific to the particular choice of base kets [2, 3]. Quite generally, we may write

$$\hat{\theta} = \hat{U} C,$$ \hspace{1cm} (1)

where $\hat{U}$ denotes a unitary operator and $C$ is complex conjugation. For simple quantum systems, the explicit form of the TR operator $\hat{\theta}$ is well known [2, 3]. Recent efforts were aimed at generalizing the TR operation to more complex systems, e.g., those having internal degrees of freedom [8].

We focus here on TR of quantum systems that carry an effective SU(2) (pseudo or real) spin degree of freedom that may be half-integer or integer. We show that SU(2) symmetry allows for two fundamentally different behaviors under TR. As TR is an antiunitary symmetry independent of the unitary symmetry elements in SU(2), it needs to be determined based on physical considerations which TR behavior applies to a particular system. This result has important consequences for effective pseudo-spin descriptions that are widely utilized. Classic examples include Schwinger’s oscillator model of angular momentum [9] (see also Sec. 3.8 in Ref. [3]), nuclear isospin [10], and the ammonia molecule [11]. More recently, the pseudo-spin concept has been ubiquitous in the context of quantum information processing [12]. Other pseudo-spin-carrying entities of current interest include the massless Dirac-electron-like quasiparticles in graphene [13] and the persistent spin helix in quasi-twodimensional semiconductor systems with fine-tuned spin-orbit couplings [14, 15]. We will discuss these particular examples and elucidate experimentally observable ramifications for the two different types of pseudo-spins.

2. Time reversal of a pseudo-spin: General properties
We start by considering the textbook example of an SU(2) angular-momentum algebra involving the three operators $\hat{J}_j$ with $j = 1, 2, 3$, satisfying the commutation relations

$$[\hat{J}_j, \hat{J}_k] = i \epsilon_{jkl} \hat{J}_l.$$ \hspace{1cm} (2)

In general, kinematically relevant physical quantities are either even or odd under TR [16]. Allowing for both possibilities for each operator $\hat{J}_j$, we write $\hat{\theta} \hat{J}_j \hat{\theta}^{-1} = \xi_j \hat{J}_j$, with $\xi_j \equiv \pm 1$. As the commutators (2) need to be preserved under TR, the three coefficients $\xi_j$ cannot be independent. Rather, they must satisfy the condition $\xi_1 \xi_2 \xi_3 = -1$, which restricts the possible TR behavior to two cases: (f) $\xi_1 = \xi_2 = \xi_3 \equiv -1$, or (b) $\xi_1 = -\xi_2 = -\xi_3 \equiv -1$, with permutations of indices allowed. Case (f) implies that all operators $\hat{J}_j$ are odd under TR, which is the behavior found for the Cartesian components of orbital and ordinary-spin angular momentum [3]. In case (b), only one of the operators $\hat{J}_j$ is odd under TR (without loss of generality chosen here to be $\hat{J}_1$), and the other two ($\hat{J}_2$ and $\hat{J}_3$) are both even. For an SU(2) invariant system of type (b), one of the Cartesian components of $\hat{J}$ is thus always distinguished by its behavior under TR.

The TR behavior associated with cases (f) and (b) generally leads to qualitatively different physical properties. For half-integer (pseudo-) spin systems, a basic feature distinguishing

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the two cases is given by the fact that \( \hat{\theta}^2 = -1 \), whereas case (b) implies \( \hat{\theta}^2 = +1 \) [3]. To prove these relations, we construct the TR operator for cases (f) and (b) in the usual representations [3], where the matrix elements of \( \hat{J}_1 \) and \( \hat{J}_3 \) are real, while those for \( \hat{J}_2 \) are imaginary. Given the general relation expressed in Eq. (1), it is only necessary to find unitary transformations \( \hat{U}_1 \) and \( \hat{U}_b \) (i.e., rotations in spin space) that yield the required transformation properties of the operators \( \hat{J}_i \). As \( \hat{J}_2 \) is odd under complex conjugation while \( \hat{J}_1 \) and \( \hat{J}_3 \) are even, it is straightforward to find \( \hat{U}_1 = \exp(i\pi\hat{J}_2) \) and \( \hat{U}_b = \exp(i\pi\hat{J}_3) \). Noting that \( \hat{C} \hat{U}_1 \hat{C} = \hat{U}_1 \), we find \( \hat{\theta}^2_1 = \hat{\theta}^2_2 \equiv \exp(2i\pi\hat{J}_3) \) amounts to a 2\( \pi \) rotation in spin space, which yields \( \hat{\theta}^2_1 = -1 \) for half-integer spin. Conversely, \( \hat{C} \hat{U}_b \hat{C} = \hat{U}^{-1}_b \) and thus \( \hat{\theta}^2_b = \hat{U}_b \hat{U}^{-1}_b \equiv +1 \).

The sign of \( \hat{\theta} \) has direct experimental consequences for the quantum interference of amplitudes for TR-related physical scenarios. Such interference plays a role, e.g., in particle interferometers [18, 19] and for the phase-coherent propagation of electrons and light through disordered media [6].

3. Physical realizations of case-(b) pseudo-spin

Whether a (pseudo-) spin degree of freedom belongs to case (f) or (b) depends on the details of the particular system under consideration. It is well-known [3] that orbital and ordinary-spin angular momentum belong to case (f). In contrast, the possibility to have the TR properties of case (b) has been under-appreciated, even though physical realizations exist. For example, it is well-known that the third Cartesian component of nuclear isospin must be even under TR by virtue of electric-charge conservation, and some implications have been considered in previous work [2, 8]. Below we further elucidate the general TR properties of type-(b) pseudo-spins using isospin as an example, and also Schwinger’s bosonic model of angular momentum [9], which is equivalent to the isotropic two-dimensional (2D) harmonic oscillator [20, 21]. Finally, we show that case (b) applies also to the persistent spin helix [14].

3.1. Nuclear isobaric spin

The isospin-1/2 model is used to describe states of the nucleon [14], with eigenstates of \( \hat{J}_3 \) being associated with the proton and neutron, respectively. The electromagnetic interaction distinguishes between the two states, and conservation of electric charge requires that all relevant states are eigenstates of \( \hat{J}_3 \). In addition, charge conservation mandates the invariance of \( \hat{J}_3 \) under TR. In the usual representation where \( \hat{J}_3 \) is real, this implies \( \hat{\theta} \hat{J}_3 \hat{\theta}^{-1} = \hat{0} \), \( \hat{J}_3 \hat{U}^{-1} = \hat{J}_3 \), i.e., \( \hat{U} \) must be a rotation around the 3-axis in isospin space. As the physically relevant isospin states are eigenstates of \( \hat{J}_3 \), \( \hat{U} \) was not specified further in previous work [2]. However, it is straightforward to verify that \( \hat{\theta}^2 = \hat{U} \hat{U}^{-1} = +1 \), i.e., isospin is an example for the type-(b) pseudo-spin.

3.2. Isotropic 2D harmonic oscillator and Schwinger model

It was realized early on [20] that the three dynamic invariants of the isotropic 2D harmonic oscillator [21] correspond to a dynamical SU(2) symmetry. Using dimensionless coordinate and momentum variables, in which the Hamiltonian reads \( H = (p_1^2 + q_1^2)/2 + (p_2^2 + q_2^2)/2 \), the three conserved quantities can be expressed as \( \hat{J}_1 = (q_1p_2 - q_2p_1)/2 \), \( \hat{J}_2 = (q_1p_2 + p_1q_2)/2 \), and \( \hat{J}_3 = (p_1^2 + q_2^2 - (p_1^2 + q_1^2))/4 \). They correspond to the orbital angular momentum of the oscillator \( \hat{J}_1 \), the energy difference for motions in the two perpendicular in-plane directions \( \hat{J}_3 \), and the phase difference between oscillations in those directions \( \hat{J}_2 \). Straightforward calculation based on the canonical commutation relations \([q_j, p_k] = i \hbar \delta_{jk} \) and \([q_j, q_k] = [p_j, p_k] = 0 \) establishes that the \( \hat{J}_j \) satisfy Eq. (2). Furthermore, the equivalence between this system and Schwinger’s bosonic model of angular momentum [3, 9] becomes apparent when the quantities \( \hat{J}_j \) are expressed in terms of creation and annihilation operators \( a^+_j = (q_j - ip_k)/\sqrt{2} \), \( a_j = (q_j + ip_k)/\sqrt{2} \) for the two 1D oscillators.

As the coordinate (momentum) components are even (odd) under TR, it follows that \( \hat{J}_1 \) is odd but both \( \hat{J}_2 \) and \( \hat{J}_3 \) are even so that this system is a realization of type (b). Even when the Schwinger-model description is applied to a general two-level system and, thus, the underlying oscillator degree of freedom is abstract, the definition of \( \hat{J}_3 \equiv (a_2^+a_2 - a_1^+a_1)/2 \) in terms of the occupation numbers of the two levels implies that \( \hat{J}_3 \) must be even under TR. Hence, many pseudo-spin models used in condensed-matter physics [22] and quantum optics [23] belong to type (b).

3.3. Persistent spin helix

The persistent spin helix is a recently discovered [14, 15] collective excitations present in certain quasi-2D semiconductor systems with fine-tuned spin-orbit couplings. In terms of second-quantized operators \( c_{k,\uparrow}^\dagger \) and \( c_{k,\downarrow} \) that, respectively, create and annihilate an electron with wave vector \( k \) and spin-up (spin-down), the following operators associated with the persistent spin helix are defined

\[
S_Q^+ = \sum_k c_{k+Q,\uparrow}^\dagger c_{k,\downarrow}, \quad S_Q^- = \sum_k c_{k,\downarrow}^\dagger c_{k+Q,\uparrow}, \quad (3a)
\]

\[
S_z = \frac{1}{2} \sum_k \left( c_{k,\uparrow}^\dagger c_{k,\downarrow} - c_{k-\downarrow}^\dagger c_{k-\uparrow} \right) \quad (3b)
\]

where \( Q \) is a function of the spin-orbit coupling strength in the system [14]. If we define \( S_z = (S_Q^+ + S_Q^-)/2 \) and \( S_y = (S_Q^+ - S_Q^-)/(2i) \), it can be shown that the components \( S_y \) obey Eq. (2).

Using the fact that both \( k \) and spin \( \uparrow, \downarrow \) are odd under TR, we find immediately \( \hat{\delta} S_Q^{-1} \hat{\theta}^{-1} = -S_z \). Similarly, we get \( \hat{\delta} S_Q^+ \hat{\theta}^{-1} = S_z \) which implies that \( S_y \) and \( S_z \) are even under TR. Hence, the SU(2) degree of freedom associated with the persistent spin helix is a type-(b) pseudo-spin.

4. Conventional and unconventional TR of 2D massless Dirac particles

In the previous section we discussed examples, where the components \( \hat{J}_j \) of the pseudo-spin were conserved, \([\hat{H}, \hat{J}_j] = 0 \) so that the TR properties of \( \hat{J}_j \) could be discussed separately
from the orbital motion. As a classic example where the (pseudo-) spin degree of freedom is coupled to the orbital motion, we now discuss particles confined to the $xy$ plane that are described by a massless Dirac Hamiltonian. Using a plane-wave basis, the Hamiltonian becomes $\hat{H}(k) = \hbar v k_\nu \sigma_\nu$, with velocity $v$ and the (pseudo-) spin operator $\sigma_\nu$

$$\sigma_\nu = x \cos \varphi_k + y \sin \varphi_k \equiv \begin{pmatrix} 0 & e^{-i\varphi_k} \\ e^{i\varphi_k} & 0 \end{pmatrix}. \quad (4)$$

Here the $\sigma_\nu$ denote the familiar Pauli matrices, and $\varphi_k$ is the angle between $k$ and the $k_\nu$ axis [see Fig. 1(a)]. The eigenvalues of $\hat{H}(k)$ are $\pm \hbar v k$, and the corresponding eigenstates are

$$|k, \pm\rangle \equiv e^{i k r} |\pm\rangle_k \equiv \frac{e^{i k r}}{\sqrt{2}} \begin{pmatrix} \pm e^{i \varphi_k/2} \\ e^{-i \varphi_k/2} \end{pmatrix}. \quad (5)$$

It is reasonable to enable a unique identification of the eigenstates by restricting $-\pi < \varphi_k \leq \pi$.

Reversal of motion should map the eigenstates of $\hat{H}(k)$ as follows:

$$\hat{\theta}_\nu |k, \pm\rangle = \eta(\nu) |k, \pm\rangle_k, \quad (6)$$

where $\eta(\nu)$ stands for an arbitrary phase, i.e., $\hat{\theta}_\nu$ should reverse the wave vector while preserving the energy. Inspection of Eq. (5) yields the relation $|\pm\rangle_{k-} = i \text{sgn}(\varphi_k) |\mp\rangle_k$, consistent with $\sigma_{k-} = -\sigma_k$. Thus $\sigma_k$ needs to be odd under the TR operation, to ensure TR invariance of $\hat{H}(k)$. For a particle confined to two spatial dimensions, this condition does not uniquely specify the TR operation. Rather, two possible scenarios exist for how the direction of $|k, \pm\rangle$ can be reversed for any given $k$. This is illustrated in Fig. 1(b). Mathematically, the two different TR operations are given by

$$\hat{\theta}_l = \exp(-i\frac{\pi}{2} \sigma_x) \exp(-i\pi \sigma_y) C \exp(i\varphi_k \sigma_z) \quad \exp(-i\pi \sigma_y) C \exp(i\varphi_k \sigma_z), \quad (7a)$$

$$\hat{\theta}_b = \exp(-i\varphi_k \sigma_z) \exp[+\text{sgn}(\varphi_k) \pi \sigma_z] C \exp(i\varphi_k \sigma_z) \quad \exp(-i\varphi_k \sigma_z) \exp[+\text{sgn}(\varphi_k) \pi \sigma_z] C. \quad (7b)$$

It is straightforward to verify that $\hat{H}(k)$ is invariant under both types of TR transformation. However, $\hat{\theta}_l$ and $\hat{\theta}_b$ can be distinguished by the way the pseudo-spin operators $\sigma_x$ and $\sigma_y$ are transformed. $[\sigma_\pm$ is the pseudo-spin in-plane component perpendicular to $\sigma_k$, see Fig. 1(a)]. More specifically, both $\sigma_x$ and $\sigma_y$ turn out to be odd under $\hat{\theta}_l$, whereas they are even under $\hat{\theta}_b$. Hence, which of the two operators $\hat{\theta}_{l,b}$ constitutes the proper TR operation for a particular system will depend on whether the actual physical quantities represented by $\sigma_x$ and $\sigma_y$ are even or odd under TR.

Before closing this Section, we briefly discuss time-reversal properties of the sublattice-related pseudo-spin degree of freedom carried by electronic quasiparticles in graphene [13]. This material consists of a sheet of carbon atoms arranged on a honeycomb lattice, with two inequivalent sublattices labeled $A$ and $B$ [Fig. 2(a)]. Its Brillouin zone is also hexagonal, with two inequivalent corner points $K$ and $K'$ [Fig. 2(b)]. Most remarkably, the energy dispersion near $K$ and $K'$ is linear, and the Fermi energy of undoped graphene is exactly at the crossing point [Fig. 2(c)]. Hence, the low-energy electronic excitations in graphene are considered to be analogs of 2D massless Dirac electrons [13, 24–28].

In situations where Umklapp processes are absent, it is tempting to treat the 2D Dirac cones at the $K$ and $K'$ valleys separately and also define an effective intra-valley time-reversal operation [27, 28]. As the pseudo-spin operator $\sigma_{\nu}$ represents the quasiparticle location on sublattice $A$ or $B$, it must be even under time reversal (as expected for a real-space position operator). $\hat{\theta}_b$ of Eq. (7b) exhibits the required property to leave $\sigma_{\nu}$ invariant (in contrast to $\hat{\theta}_l$), suggesting it to be a proper intra-valley time-reversal operator. However, it should be noted that the ordinary TR for Bloch electrons in graphene is given by $\hat{\theta} = C$ which couples the two valleys [28]. In order to apply the discussion of this Section to graphene, a restriction of anti-unitary operators to individual valleys needs to be formulated.

5. Observable signatures of the two types of pseudo-spin

Whether a particular realisation of pseudo-spin belongs to type (f) or (b) is not a purely academic question, as their different TR properties affect physical observables. For example, in the case of 2D Dirac particles considered in the previous Section, a (possibly random) potential $V(r)\sigma_z$ does not break $\hat{\theta}_b$-TR symmetry, whereas such a potential will break the $\hat{\theta}_l$-TR symmetry [29]. As a result, the level statistics of chaotic quantum dots formed by a non-integrable mass-confinement of 2D Dirac particles will be different in the two cases [29]. While this example is specific to the case of 2D Dirac particles, we
will now discuss a more general observable difference exhibited by half-integer pseudo-spin particles of type-(f) and (b) that are scattered by a spin-independent random potential but are free otherwise. The quantum interference of TR-related backscattering amplitudes turns out to be different for the two pseudo-spin types and can thus serve to distinguish them experimentally.

We denote scattering states of the particle by $|k, s\rangle$, where $k$ denotes the wave vector and $s$ is the pseudo-spin quantum number w.r.t. some specific basis. The probability amplitude for a particular backscattering process involving $n$ scattering events due to a disorder potential is then proportional to

$$
\mathcal{A}_{k_1, s_1, \ldots, k_n, s_n} = \langle -k, s|k_n, s_n\rangle \langle k_n, s_n|k_{n-1}, s_{n-1}\rangle \ldots \langle k_2, s_2|k_1, s_1\rangle\langle k_1, s_1|k, s\rangle. 
$$

(8)

In the typical situation where disorder potentials are invariant under TR, each such process has a “partner” process

$$
\mathcal{A}_{k_1, s_1, \ldots, k_n, s_n} = \langle -k, s|\hat{\theta}(k_1, s_1)\rangle\langle \hat{\theta}(k_1, s_1)|\hat{\theta}(k_2, s_2)\rangle \ldots \langle \hat{\theta}(k_{n-1}, s_{n-1})|\hat{\theta}(k_{n-1}, s_{n-1})\rangle\langle \hat{\theta}(k_n, s_n)|k, s\rangle, 
$$

(9)

where scattering occurs in time-reversed order. Using the relations $|\hat{\theta}(a)| = (\hat{\theta}\hat{\theta}|a\rangle$ and $|\hat{\theta}(k, s)| = |-k, s\rangle$, we find

$$
\mathcal{A}_{k_1, s_1, \ldots, k_n, s_n} = \langle -k, s|\hat{\theta}(k_1, s_1)|\hat{\theta}(k_2, s_2)\rangle \ldots \langle \hat{\theta}(k_{n-1}, s_{n-1})|\hat{\theta}(k_n, s_n)|k, s\rangle
$$

$$
= \text{sgn}(\hat{\theta}) \mathcal{A}_{k_1, s_1, \ldots, k_n, s_n}. 
$$

(10)

The total probability for backscattering of a particle is the modulus square of the sum over the probability amplitudes of all possible back-scattering processes. If the sign of $\hat{\theta}$ is positive (negative), scattering processes related by TR will interfere constructively (destructively), leading to reduced (enhanced) particle transmission through the medium. Thus we suggest that quantum-coherent transport provides an avenue for distinguishing between half-integer type-(f) and type-(b) pseudo-spins, because $\hat{\theta}_{\text{f}} = -\hat{\theta}_{\text{b}} \equiv -1$. Direct observation of the backscattering probability would facilitate such an experimental distinction.

6. Conclusions

We have shown that (pseudo-) spin degrees of freedom can be classed into two types according to their time-reversal properties. For type (f), which includes ordinary spin angular momentum, all three spin components are odd under time reversal. For type (b), only one of the components is odd under time reversal while the remaining two are even. This case includes nuclear isospin and the dynamic SU(2) symmetry of the 2D isotropic harmonic oscillator.

As an example of a system for which (pseudo-) spin and orbital motion are coupled, we discussed time reversal of massless Dirac particles confined to move in two spatial dimensions. It was found that the dynamics of the system again allows for time-reversal operations of the two types (f) and (b). Only by considering the properties of additional observables represented, e.g., by the $z$ component of pseudo-spin is it possible to uniquely determine the form of the time-reversal operation.

Which type of time-reversal operation is realised in a particular system has measurable consequences. For example, whether itinerant particles with half-integer (pseudo-) spin belong to type (f) or (b) manifests itself in an experimentally observable way by the relative sign of probability amplitudes associated with time-reversal-related back-scattering scenarios. This and several more observable ramifications associated with randomness/chaotic dynamics arise because the squared anti-unitary operators associated with the time-reversal transformation in the two cases differ by their sign.

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