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Article

Quantum Correlations under Time Reversal and Incomplete Parity Transformations in the Presence of a Constant Magnetic Field

Paolo De Gregorio ^{1,*}, Sara Bonella ² and Lamberto Rondoni ^{1,3,4}

¹ Dipartimento di Scienze Matematiche, Politecnico di Torino, Corso Duca degli Abruzzi 24, I-10129 Torino, Italy

² Centre Européen de Calcul Atomique et Moléculaire (CECAM), École Polytechnique Fédérale de Lausanne, Batochime, Avenue Forel 2, 1015 Lausanne, Switzerland; sara.bonella@epfl.ch

³ Graphene@PoliTO Lab, Politecnico di Torino, Corso Duca degli Abruzzi 24, I-10129 Torino, Italy; lamberto.rondoni@polito.it

⁴ Istituto Nazionale di Fisica Nucleare, Sezione di Torino, Via P. Giura 1, I-10125 Torino, Italy

* Correspondence: paolo.degregorio@polito.it; Tel.: +39-011-090-7538

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Abstract: We derive the quantum analogues of some recently discovered symmetry relations for time correlation functions in systems subject to a constant magnetic field. The symmetry relations deal with the effect of time reversal and do not require—as in the formulations of Casimir and Kubo—that the magnetic field be reversed. It has been anticipated that the same symmetry relations hold for quantum systems. Thus, here we explicitly construct the required symmetry transformations, acting upon the relevant quantum operators, which conserve the Hamiltonian of a system of many interacting spinless particles, under time reversal. Differently from the classical case, parity transformations always reverse the sign of both the coordinates and of the momenta, while time reversal only of the latter. By implementing time reversal in conjunction with ad hoc “incomplete” parity transformations (i.e., transformations that act upon only some of the spatial directions), it is nevertheless possible to achieve the construction of the quantum analogues of the classical maps. The proof that the mentioned symmetry relations apply straightforwardly to quantal time correlation functions is outlined.

Keywords: time correlation functions; time reversal; parity; quantum symmetry transformations

1. Introduction

Microscopic time reversibility is a key precept in Physics. Its usefulness is not limited to discussions around causality or about its relation with macroscopic irreversibility: it is also a useful tool to derive relations regarding dynamical observables such as transport coefficients. Since Casimir first discussed Onsager’s relations of microscopic reversibility [1], it has become customary to refer to time correlation functions in the presence of a magnetic field in a different manner than their counterparts in the absence of it [2,3]. It is typically stated or implied that any time reversal symmetry is associated with a reversal of the magnetic field. Other symmetries which emancipate one from that obligation have not been discussed until very recently [4]. Kubo [5–7] derived classical and quantal symmetry relations for time correlation functions in systems subjected to an external constant magnetic field. These relations all involve time- and magnetic field-reversal. Concisely written, they are expressed as $\langle X(0) \cdot Y(t) \rangle_{\mathbf{B}} = \eta_X \eta_Y \langle X(0) \cdot Y(-t) \rangle_{-\mathbf{B}}$, where \cdot stands for canonical multiplication in classical systems, and for appropriately specified combinations of the observable operators qualifying X and Y in quantum systems. η_X and η_Y are signatures (i.e., they take up the values ± 1), specifying the effect of the reversal of time, of the momenta, and of the magnetic field on the observables X and Y , respectively.

The association of magnetic field reversal with time reversal is usually interpreted as signifying the odd character of the field itself, with respect to the underlying symmetry transformation. This is pacific if one considers time reversal acting on the Universe as a whole, so that the external magnetic field is reversed as well. It is however arbitrary in character when time reversal is only considered to pertain to a certain specific subsystem of interest, with respect to which the magnetic field is an external force. The traditional approach of Kubo, while formally correct, forces one to consider symmetry relations only between pairs of subclasses of systems, each item in one class having the external magnetic field in the opposite direction to that of each item in the other class. As mentioned above, however, it was recently shown that generalized time reversal symmetries between subsystems subject to the same magnetic field can be established [4]. Interestingly, these symmetries relate observables within the *same* system. As discussed in more detail in the next section, it suffices to transform only some of the coordinates and momenta in some prescribed manner. Thus, in [4] it was shown that for classical systems $\langle X(0)Y(t) \rangle_{\mathbf{B}} = \eta_X \eta_Y \langle X(0)Y(-t) \rangle_{\mathbf{B}}$, now η_X, η_Y being the signatures with respect to the particular symmetry transformations which have been selected. The only requirement is that the peculiar transformation associated with time reversal leaves the microscopic dynamics invariant. Now the correlation relations involve solely the time evolution of the system's own time-dependent observables, and therefore bear physical relations between its constituents. They no more involve—as in the previous formulations—a purported one-to-one matching between the constituents of two systems, interacting selectively with two magnetic fields pointing in opposite directions.

The above observation may have some consequences when one considers statistical averages or fluctuation relations in many-body systems, interacting among themselves and with a constant external magnetic field. In general, when many trajectories are possible within a given macroscopic ensemble, any symmetry may imply the possibility of establishing a one-to-one correspondence between “forward” and “backward” trajectories. Weighing each trajectory with the probability distribution of its initial value, one arrives at estimating the relative probabilities of finding the system in two distinct macroscopic states [8,9].

In [4] it was anticipated that that the newly established symmetry relations could be extended to the quantum case. Indeed, care must only be taken to deal with the interlacing of coordinates and momenta operators with respect to parity. It is then possible to extend the classical result to the quantum case, as we show in this paper. It also emerges that the recipe for finding the entire class of admissible transformations is neatly established by requiring the invariance of the quantum Hamiltonian. Only the case of a time-independent Hamiltonian and a system of spineless particles has been considered here.

2. From the Classical Result to a Quantum System

Let us consider a system of N spinless particles of mass m_i and charge q_i in the presence of a constant magnetic field \mathbf{B} . In the case of classical mechanics, in [4] the existence of a length-conserving, time-reversing symmetry transformation \mathcal{M} was proven, such that

$$\langle \Phi(0)\Psi(t) \rangle_{\mathbf{B}} = \eta_{\Phi}\eta_{\Psi} \langle \Phi(0)\Psi(-t) \rangle_{\mathbf{B}} \quad (1)$$

under the transformation. Φ and Ψ are any two observables, respectively with signatures $\eta_{\Phi} = \pm 1$ and $\eta_{\Psi} = \pm 1$ under \mathcal{M} . The result complements that of Kubo [5–7], who far earlier found that similar general correlation relations hold for (concurrent) time- and \mathbf{B} -reversal symmetries. The peculiarity of (1) is that it directly permits the formal derivation of some equilibrium and nonequilibrium properties within a single system (e.g., fluctuation relations), via the association of trajectories which are pair-wise invariant under time reversal, even if the field \mathbf{B} is not reversed [9]. Furthermore, the map \mathcal{M} is not unique [10] and this straightforwardly implies constraints on time correlation functions, since combining the maps produces certain self-antisymmetric relations.

In [4], it was also conjectured that in the context of quantum mechanics, a map operating similarly to \mathcal{M} would produce the same type of relations as in (1), provided one uses the appropriate quantal correlation functions. The need to use certain appropriate correlation functions in quantum systems stems from the fact that Φ and Ψ may not commute in general and, by consequence, correlators as in (1) may not be real-valued, the averaged operator being nonhermitian. This is a limitation if one wants to associate the correlators themselves with observable quantities. Further, parity operators work differently from the classical case, where momentum and position are independent, as the quantum momentum is a position-dependent operator in coordinates space. Here, we set out to explicitly prove the above-mentioned conjecture, providing a simple recipe for exhausting the alternative choices of map.

We start by briefly reviewing the classical case [4]. To fix our ideas, \mathbf{B} is parallel to z , $\mathbf{B} = B \mathbf{e}_z$ and the vector potential satisfies $2\mathbf{A}(\mathbf{r}) = B(-y \mathbf{e}_x + x \mathbf{e}_y)$. The map \mathcal{M} is defined as:

$$\mathcal{M} : (x, y, z, p^x, p^y, p^z, t) \mapsto (x, -y, z, -p^x, p^y, -p^z, -t). \quad (2)$$

Given the particles occupying positions \mathbf{r}_i and defining $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$, the equations of motion are derived from the classical Hamiltonian:

$$\mathcal{H} = \sum_{i=1}^N \frac{(\mathbf{p}_i - q_i \mathbf{A}(\mathbf{r}_i))^2}{2m_i} + \frac{1}{2} \sum_{i \neq j}^{1,N} U(|\mathbf{r}_{ij}|) \quad (3)$$

and they read, after defining $\omega_i = \frac{q_i B}{2m_i}$ and the α component ($\alpha = x, y, z$) of the force on particle i ,

$$F_i^\alpha = -\frac{\partial}{\partial \alpha_i} \sum_{j \neq i}^N U(|\mathbf{r}_{ij}|):$$

$$\begin{aligned} \dot{x}_i &= \frac{p_i^x}{m_i} + \omega_i y_i, & \dot{p}_i^x &= F_i^x + \omega_i (p_i^y - m_i \omega_i x_i), \\ \dot{y}_i &= \frac{p_i^y}{m_i} - \omega_i x_i, & \dot{p}_i^y &= F_i^y - \omega_i (p_i^x + m_i \omega_i y_i), \\ \dot{z}_i &= \frac{p_i^z}{m_i}, & \dot{p}_i^z &= F_i^z. \end{aligned} \quad (4)$$

The map \mathcal{M} leaves the dynamics in (4) invariant.

To build the quantum notation, we start by noting the effect of the relevant transformations on the single-particle quantum operators. From now on, all variables are to be understood as quantum operators. Time reversal is represented by an anti-unitary \mathcal{T} transformation [11,12], satisfying:

$$\mathcal{T} \alpha_i \mathcal{T}^{-1} = \alpha_i, \quad \mathcal{T} p_i^\alpha \mathcal{T}^{-1} = -p_i^\alpha, \quad (\alpha = x, y, z); \quad \mathcal{T} i \mathcal{T} = -i. \quad (5)$$

Parity restricted to the direction β of space entails the following ($\alpha, \beta = x, y, z$):

$$\mathcal{P}_\beta \alpha_i \mathcal{P}_\beta^{-1} = (1 - 2\delta_{\alpha\beta}) \alpha_i, \quad \mathcal{P}_\beta p_i^\alpha \mathcal{P}_\beta^{-1} = (1 - 2\delta_{\alpha\beta}) p_i^\alpha, \quad \mathcal{P}_\beta i \mathcal{P}_\beta^{-1} = i. \quad (6)$$

Here, $\delta_{\alpha\beta} = 1$ if $\alpha = \beta$ and $\delta_{\alpha\beta} = 0$ otherwise. Thus, for example, \mathcal{P}_x acts as the identity with respect to the y_i and z_i coordinate operators and the p_i^y and p_i^z momentum operators, while it reverses the sign of both x_i and p_i^x . The latter effect on momenta distinguishes a quantum system from a classical system and it reflects the fact that the quantum momentum in real space is a differential operator with respect to the homologous coordinate. By introducing (6), one is able to consider incomplete parity transformations; i.e., transformations that emulate parity, but only with respect to some assigned direction or directions. To incorporate all incomplete parity transformations, one can thus also define:

$$\mathcal{P}_{\alpha\beta} = \mathcal{P}_\alpha \mathcal{P}_\beta. \quad (7)$$

The complete parity—or simply parity—is trivially given by $\mathcal{P} = \mathcal{P}_x \mathcal{P}_y \mathcal{P}_z$. With \mathcal{P}_α and $\mathcal{P}_{\alpha\beta}$, combined eventually with \mathcal{T} (which commute with all \mathcal{P}_* 's), one is able to investigate various symmetries in quantum Hamiltonian systems. For example, the map \mathcal{M} in (2) has the following counterpart in quantum mechanics:

$$\mathcal{M} \longmapsto \mathcal{M}_y = \mathcal{P}_y \mathcal{T}. \quad (8)$$

One more remark is in order. Since \mathcal{T} is anti-unitary, it follows [11,12] that the only two alternative possibilities are

$$\mathcal{T}^{-1} = \eta_{\mathcal{T}} \mathcal{T}, \quad (\eta_{\mathcal{T}} = \pm 1), \quad (9)$$

where $\eta_{\mathcal{T}} = 1$ for particles without internal degrees of freedom.

3. Invariance of the Quantum Hamiltonian

The quantum mechanical transcription of Equation (3) gives the quantum Hamiltonian as soon as any variable is replaced by the corresponding quantum operator. In the Coulomb gauge, Equation (3) now reads:

$$\mathcal{H} = \sum_{i=1}^N \left(\frac{\mathbf{p}_i^2}{2m_i} - \frac{q_i}{m_i} \mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p}_i + \frac{q_i^2}{2m_i} \mathbf{A}^2(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{i \neq j}^{1,N} U(|\mathbf{r}_{ij}|) \quad (10)$$

and is further simplified by the above-specified alignment of the magnetic field $\mathbf{B} = B \mathbf{e}_z$, and form of the vector potential, $2\mathbf{A}(\mathbf{r}) = B(-y \mathbf{e}_x + x \mathbf{e}_y)$,

$$\mathcal{H} = \sum_{i=1}^N \left(\frac{\mathbf{p}_i^2}{2m_i} + \frac{q_i B}{2m_i} y_i p_i^x - \frac{q_i B}{2m_i} x_i p_i^y + \frac{q_i^2 B^2}{8m_i} (x_i^2 + y_i^2) \right) + \frac{1}{2} \sum_{i \neq j}^{1,N} U(|\mathbf{r}_{ij}|). \quad (11)$$

Now note that:

$$\begin{aligned} \mathcal{M}_y x_i \mathcal{M}_y^{-1} &= x_i; & \mathcal{M}_y y_i \mathcal{M}_y^{-1} &= -y_i; & \mathcal{M}_y z_i \mathcal{M}_y^{-1} &= z_i; \\ \mathcal{M}_y p_i^x \mathcal{M}_y^{-1} &= -p_i^x; & \mathcal{M}_y p_i^y \mathcal{M}_y^{-1} &= p_i^y; & \mathcal{M}_y p_i^z \mathcal{M}_y^{-1} &= -p_i^z; \\ \mathcal{M}_y \mathbf{A}(\mathbf{r}_i) \mathcal{M}_y^{-1} &= B(y_i \mathbf{e}_x + x_i \mathbf{e}_y)/2. \end{aligned} \quad (12)$$

As for higher-order operators:

$$\begin{aligned} \mathcal{M}_y \mathbf{p}_i^2 \mathcal{M}_y^{-1} &= \mathbf{p}_i^2; & \mathcal{M}_y \mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p}_i \mathcal{M}_y^{-1} &= \mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p}_i; \\ \mathcal{M}_y \mathbf{A}^2(\mathbf{r}_i) \mathcal{M}_y^{-1} &= \mathbf{A}^2(\mathbf{r}_i); & \mathcal{M}_y U(|\mathbf{r}_{ij}|) \mathcal{M}_y^{-1} &= U(|\mathbf{r}_{ij}|). \end{aligned} \quad (13)$$

It follows that the Hamiltonian is invariant with respect to the transformation \mathcal{M}_y ,

$$\mathcal{M}_y \mathcal{H} \mathcal{M}_y^{-1} = \mathcal{H}. \quad (14)$$

This is a necessary and sufficient condition for the dynamics of a time-independent Hamiltonian to be invariant, and one could also readily inspect its character by applying the operator \mathcal{M}_y to the evolution of the wave function ψ ; i.e., $i\partial_t \psi - \mathcal{H}\psi = 0$,

$$\mathcal{M}_y (i\partial_t - \mathcal{H}) \psi = (-i\partial_t - \mathcal{H}) \mathcal{M}_y \psi = 0. \quad (15)$$

Therefore $\psi' = \mathcal{M}_y \psi$ is a solution of the equation $(-i\partial_t - \mathcal{H})\psi' = 0$, which is precisely the original Schrodinger equation, after the replacement $t \rightarrow -t$.

Equations (3), (10) and (11) are alternative representations in the case of \mathbf{B} aligned with \mathbf{e}_z , and allow one to derive the transformations which leave the Hamiltonian invariant. The term which is problematic when time reversal is considered is, for example, $\mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p}_i$ in (10). Traditionally, to attain invariance of \mathcal{H} , one observes that \mathcal{T} reverses all \mathbf{p}_i 's, and therefore the magnetic field must also be reversed (and thus inversion of \mathbf{A} follows). An additional complete parity transformation would only flip all the coordinates and all the momenta, without changing the relative signs of the momenta with respect to the magnetic field. The only way to obtain a transformation that preserves the sign of B and also reverses time is that $\mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p}_i$ be invariant. Along with $\mathcal{M}_y = \mathcal{P}_y \mathcal{T}$, then also $\mathcal{M}_x = \mathcal{P}_x \mathcal{T}$, $\mathcal{M}_{yz} = \mathcal{P}_{yz} \mathcal{T}$, and $\mathcal{M}_{xz} = \mathcal{P}_{xz} \mathcal{T}$ comply with the requirement. It is noted that this is a definitive assessment in the quantum formalism, which is distinct from the classical requirement that Equation (4) be invariant, albeit the two approaches may lead to reciprocally consistent conclusions.

4. Correlation Functions

For brevity, we denote as \mathcal{M} any of the four aforementioned quantum transformations, which leave the magnetic field unchanged and with respect to which the Hamiltonian is invariant. Suppose that

$$\mathcal{M} \Phi \mathcal{M}^{-1} = \eta_\Phi \Phi \quad \text{and} \quad \mathcal{M} \Psi \mathcal{M}^{-1} = \eta_\Psi \Psi, \quad (\eta_\Phi, \eta_\Psi = \pm 1). \quad (16)$$

We consider the time correlator

$$\langle \Phi(0) \Psi(t) \rangle = \text{Tr} [\rho \Phi(0) \Psi(t)]. \quad (17)$$

ρ is the density operator generating the implied equilibrium probability measure. Notice that (17) could be non-observable, since Φ and Ψ may not commute, which implies that $\Phi(0)\Psi(t)$ be nonhermitian for finite times. It is, however, mathematically well-defined.

We have:

$$\begin{aligned} \langle \Phi(0) \Psi(t) \rangle &= \text{Tr} [\rho \Phi(0) e^{\frac{i\mathcal{H}t}{\hbar}} \Psi(0) e^{-\frac{i\mathcal{H}t}{\hbar}}] = \text{Tr} [\rho \Phi(0) e^{\frac{i\mathcal{H}t}{\hbar}} \mathcal{M}^{-1} \mathcal{M} \Psi(0) \mathcal{M}^{-1} \mathcal{M} e^{-\frac{i\mathcal{H}t}{\hbar}}] \\ &= \eta_\Psi \text{Tr} [\rho \Phi(0) e^{\frac{i\mathcal{H}t}{\hbar}} \mathcal{M}^{-1} \Psi(0) \mathcal{M} e^{-\frac{i\mathcal{H}t}{\hbar}}] = \eta_\Psi \text{Tr} [\rho \Phi(0) \mathcal{M}^{-1} e^{-\frac{i\mathcal{H}t}{\hbar}} \Psi(0) e^{\frac{i\mathcal{H}t}{\hbar}} \mathcal{M}] \\ &= \eta_\Psi \text{Tr} [\rho \mathcal{M} \Phi(0) \mathcal{M}^{-1} e^{-\frac{i\mathcal{H}t}{\hbar}} \Psi(0) e^{\frac{i\mathcal{H}t}{\hbar}}] = \eta_\Phi \eta_\Psi \text{Tr} [\rho \Phi(0) e^{-\frac{i\mathcal{H}t}{\hbar}} \Psi(0) e^{\frac{i\mathcal{H}t}{\hbar}}] = \eta_\Phi \eta_\Psi \langle \Phi(0) \Psi(-t) \rangle. \end{aligned}$$

In addition to (16), we have used the following identities:

$$\mathcal{M} e^{-\frac{i\mathcal{H}t}{\hbar}} = e^{\frac{i\mathcal{H}t}{\hbar}} \mathcal{M}, \quad e^{\frac{i\mathcal{H}t}{\hbar}} \mathcal{M}^{-1} = \mathcal{M}^{-1} e^{-\frac{i\mathcal{H}t}{\hbar}}, \quad \text{Tr} [\rho A \mathcal{M}] = \text{Tr} [\rho \mathcal{M} A], \quad (18)$$

the first two of which express the invariance of \mathcal{H} under the anti-unitary transformation \mathcal{M} and account for the anti-hermitian property of the time reversal operator—see Equations (5) and (8), the latter following from the invariance of the trace under cyclic permutation of operators, in addition to \mathcal{M} commuting with the equilibrium density operator, assumed to depend on the Hamiltonian. The first two identities in (18) have a dynamical interpretation. For example, in layman terms, the first of them expresses the possibility of inferring the state of a system which progressed from some time $-t$ in the past and was then transformed by \mathcal{M} by just applying \mathcal{M} to the actual state and letting it evolve for a time t in the future. One may also express the time reversal symmetries here illustrated as one way to obtain the state in the past that has produced the present state, by evolving forward in time the state obtained by applying the symmetry operator to the present state, and then applying the symmetry

operator at the end of that evolution. After all, it is not possible to travel backward in time, as far as we know.

In the case of $\Psi = \Phi$, it trivially follows that

$$\langle \Phi(0)\Phi(t) \rangle = \langle \Phi(0)\Phi(-t) \rangle,$$

which is now a relation between two observable averages.

Following Kubo, we may readily write for the symmetrized correlator $\langle X, Y \rangle = \langle XY \rangle + \langle YX \rangle$:

$$\langle \Phi(0), \Psi(t) \rangle = \eta_{\Phi} \eta_{\Psi} \langle \Phi(0), \Psi(-t) \rangle$$

The proof is trivial.

Kubo also defines

$$\langle \Phi(0); \Psi(t) \rangle = \frac{1}{\beta} \int_0^{\beta} d\lambda \operatorname{Tr} [\rho e^{\lambda \mathcal{H}} \Phi(0) e^{-\lambda \mathcal{H}} \Psi(t)], \quad (19)$$

which is also real, as is the symmetrized one, because it is the average of a hermitian operator.

Now, reiterating the proof in (18) after replacing $\Phi(0)$ with $e^{\lambda \mathcal{H}} \Phi(0) e^{-\lambda \mathcal{H}}$, it is straightforward to write:

$$\begin{aligned} \langle \Phi(0); \Psi(t) \rangle &= \frac{1}{\beta} \int_0^{\beta} d\lambda \operatorname{Tr} [\rho e^{\lambda \mathcal{H}} \Phi(0) e^{-\lambda \mathcal{H}} \Psi(t)] \\ &= \frac{\eta_{\Phi} \eta_{\Psi}}{\beta} \int_0^{\beta} d\lambda \operatorname{Tr} [\rho e^{\lambda \mathcal{H}} \Phi(0) e^{-\lambda \mathcal{H}} \Psi(-t)] = \eta_{\Phi} \eta_{\Psi} \langle \Phi(0); \Psi(-t) \rangle. \end{aligned} \quad (20)$$

We point out that it is a simple exercise, starting from the quantum Hamiltonian (3) and choosing the Landau gauge $\mathbf{A}(\mathbf{r}) = -B y \mathbf{e}_x$, or alternatively $\mathbf{A}(\mathbf{r}) = B x \mathbf{e}_y$, to obtain again the result. Indeed, the said Hamiltonian is notoriously gauge invariant, which implies that its wave functions absorb a gauge transformation by acquiring a local gauge phase; i.e., multiplication by a unitary operator (here time-independent). A physical operator must undergo the same unitary transformation for every new choice of the vector potential. Notice that $\mathcal{P}_y \mathcal{T}$ correctly transforms each quadratic term in (3) in the chosen gauges, acting always on the generalized momenta.

5. Conclusions

By providing a systematic procedure to identify the quantum analogue of the generalized time reversal symmetries introduced in [4] for classical systems, we have proved that well-defined signature properties for quantum time correlations can be derived, as conjectured in previous work. More precisely, Equation (20) has been proved for systems whose equilibrium distribution depend only on the Hamiltonian (10). We have found a way to systematically identify the transformations for which (20) is valid. The result implies that for spinless particles obeying the time-independent Hamiltonian (10), there exist time-reversal symmetry transformations which do not require inversion of the magnetic field. The notion that any external magnetic field is an intrinsically odd quantity for any time-reversal transformation should be reviewed. The present work does not address the case of particles with spin interacting with the magnetic field, or the case of time-dependent Hamiltonians.

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