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Topological Invariants in Fermi Systems with Time-Reversal Invariance

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We discuss topological invariants for Fermi systems that have time-reversal invariance. The TKN^2 integers (first Chern numbers) are replaced by second Chern numbers, and Berry's phase becomes a unit quaternion, or equivalently an element of SU(2). The canonical example playing much the same role as spin $\frac{1}{2}$ in a magnetic field is spin $\frac{3}{2}$ in a quadrupole electric field. In particular, the associated bundles are nontrivial and have ± 1 second Chern number. The connection that governs the adiabatic evolution coincides with the symmetric SU(2) Yang-Mills instanton.

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Much interest has focused recently on topological and geometric invariants in eigenvalue perturbation theory, namely on TKN^2 integers[1,2] and on Berry's phase.[3,4] The folk wisdom is that nontrivial values of these invariants require broken time-reversal invariance such as occurs in a magnetic field. This belief is correct in the sense that if all Hamiltonians can be made simultaneously real, the invariants vanish. But such simultaneous reality is a feature of time-reversal invariance for integer spins, i.e., Bose systems only. Our goal here is to discuss the rich structure present for time-reversal–invariant half-odd-integer spins, i.e., Fermi systems. Additional details will appear in Ref. 5. Non-Abelian phases in Kramers degenerate systems have previously been considered in Ref. 6.

Let **J** be the angular momentum operator, which is, of course, odd under time reversal. In the usual representation (with J_x and J_z real and J_y imaginary) time reversal, which we call T, may be implemented by the product of complex conjugation and rotation about the y axis by π. This is in fact the only antiunitary operator, up to phases, that reverses **J**. In representations where J is half-odd integral, rotation by 2π is -1, and so $T^2=-1$.

This holds in general. That is, in Fermi systems with time-reversal invariance, there exists an antiunitary operator T which commutes with the Hamiltonian (or family of Hamiltonians if some external parameters are varied) and obeys $T^2=-1$. Since T anticommutes with multiplication by i, it gives the Hilbert space a quaternionic structure,[7,8] if we think of T as multiplication by j and iT as multiplication by k.

H is time-reversal invariant if it commutes with T.[9] This says that H is Hermitian in the quaternionic sense. The eigenspaces are quaternionic vector spaces and so are even dimensional as complex vector spaces. Kramers' degeneracy[7] follows immediately from this structure. An eigenvalue is called *quaternionically simple* if it has the minimum degeneracy consistent with Kramers, namely double, degeneracy in the sense of a complex Hilbert space.

As for complex Hermitian matrices, where generically all eigenvalues are simple in the complex sense, the eigenvalues of quaternionic Hermitian matrices are generically simple in the quaternionic sense. (The usual definition but with complex conjugate replaced by quaternionic conjugate.) Whereas in the complex Hermitian case eigenvalue crossings have codimension 3, in the quaternionic Hermitian case they have codimension 5. Simple parametric counting via Wigner and von Neumann[10] yields these numbers. Codimension 5 means that, generically, there are no level crossings on four-dimensional surfaces.

What we have said so far is not new, and is presented for background. In the complex case, a basic role is played by the homotopy groups of $M_n(\mathbb{C})$, the space of nondegenerate, complex Hermitian $n\times n$ matrices. This space is homotopic to the quotient $U(n)/[U(1)\times\cdots\times U(1)]$ of the unitary matrices. As shown in Ref. 2, $\pi_2[M_n(\mathbb{C})]=\mathbb{Z}^{n-1}$, which reflects the fact that there is a TKN^2 integer associated with each eigenvalue, and the integers satisfy a zero sum rule.

The quaternionic analog is $M_n(\mathbb{H})$, the nondegenerate quaternionic Hermitian $n\times n$ matrices, which is homotopic to the quotient $\mathrm{Sp}(n)/[\mathrm{Sp}(1)\times\cdots\times\mathrm{Sp}(1)]$ of the unitary symplectic matrices by the diagonal unitary symplectic matrices.[9] Now $\pi_j[M_n(\mathbb{H})]=0$ for $j=1,2,3$ and $\pi_4[M_n(\mathbb{H})]=\mathbb{Z}^{n-1}$. These results follow from the homotopy exact sequences. $M_n(\mathbb{H})$ turns out to have a richer homotopy than $M_n(\mathbb{C})$ for the simple reason that $\mathrm{Sp}(1)\sim S^3$ has a richer homotopy than $U(1)\sim S^1$, so unlike the complex case, there are higher homotopy invariants in the quaternionic case.[5]

The TKN^2 integers associated to a map of S^2 to $M_n(\mathbb{C})$ can be computed as the integral of the first Chern two-form ω_1. In terms of the projection $P(Q)$ onto the one-dimensional eigenspace for $H(Q)$ depending on parameter Q, the curvature Ω is given by $\Omega=iP(dP\wedge dP)$, and

$$\omega_1=\frac{1}{2\pi}\mathrm{Tr}(\Omega).$$

The TKN^2 numbers are the first Chern numbers, $C_1\equiv\int_{S^2}\omega_1$, where S^2 is a closed two-surface in parameter space. For the canonical example $H(B)=\mathbf{J}\cdot\mathbf{B}$, $C_1=2m$, where m is the azimuthal quantum number. Clearly, if $H(Q)$ commutes with T, then $\omega_1\equiv 0$.

In the quaternionic case, the basic object is the second Chern four-form (in this context more appropriately called the first symplectic Pontryagin form[11])

$$\omega_2=\frac{1}{8\pi^2}[\mathrm{Tr}(\Omega^2)-\mathrm{Tr}(\Omega)^2]=\frac{1}{8\pi^2}\mathrm{Tr}(\Omega^2),$$

so that, for example, if Q parametrizes points in S^4, then the second Chern integer is given by

$$C_2=\int_{S^4}\omega_2. \tag{1}$$

As in the complex case, solving the Schrödinger equation adiabatically (or in any other smooth way that is guaranteed to return to the initial state[12]) produces a holonomy identical to the natural one induced by the metric on the Hilbert space on the bundle of eigenspaces.[4] In the complex case, this holonomy is given by a complex number of magnitude one—the Berry's phase. In the quaternionic case it is given by a unit quaternion, or equivalently by an element of SU(2). In the general twofold-degenerate case considered by Wilczek and Zee,[3] the holonomy is an element of U(2).

These rather abstract considerations are made concrete in a set of elementary examples. Since $\mathbf{J}$ is odd under T, the simplest time-reversal–invariant Hamiltonian is

$$H(Q)\equiv\sum_{mn}Q_{mn}J_mJ_n, \tag{2}$$

with Q a real symmetric second-rank tensor, which may be taken traceless. The space of such tensors is a five-dimensional real vector space, with an invariant inner product given by $\langle Q,Q'\rangle\equiv\frac{3}{2}\mathrm{Tr}(QQ')$, where the trace is taken as the trace of linear operators on $\mathbb{R}^3$. A standard orthonormal basis Q_α, $\alpha=0,\ldots,4$, can be defined such that, using $e_\alpha=H(Q_\alpha)$, $e_0\equiv J_z^2-J^2/3$, $e_1\equiv 3^{-1/2}(J_xJ_z+J_zJ_x)$, $e_2\equiv 3^{-1/2}(J_yJ_z+J_zJ_y)$, $e_3\equiv 3^{-1/2}(J_x^2-J_y^2)$, and $e_4\equiv 3^{-1/2}(J_xJ_y+J_yJ_x)$.

While this example looks specialized, by the Wigner-Eckart theorem it will apply to any spin-J multiplet perturbed by a second-rank tensor. For example, our Berry's phase calculation below will be relevant to any spin-atomic $\frac{3}{2}$ level under perturbation by an electric quadrupole.

At $Q=0$, $H(Q)=0$ is obviously highly degenerate. One can show that for $Q\neq 0$ all levels are simple in the quaternionic sense, i.e., only doubly degenerate in the complex sense.[5] If we take for S^4 in Eq. (1) the unit sphere in the space of tensor operators, i.e., $\frac{3}{2}\mathrm{Tr}(Q^2)=1$, all the $J+\frac{1}{2}$ energy levels have well defined second Chern integers, satisfying a zero sum rule. Moreover, a simple argument shows that C_2 of the nth eigenvalue is $-C_2$ of the $(J+\frac{3}{2}-n)$th eigenvalue. This is in some ways like the situation discussed by Berry,[3] except that for $J>\frac{3}{2}$, there is not enough symmetry to facilitate a simple calculation of the C_2's.

The case $J=\frac{3}{2}$ is basic and has some remarkable symmetries, as we will explain. The sense that it is basic is that, as in Ref. 4, the generic situation for quaternion degeneracies as one varies five parameters is twofold degeneracy removed to first order. Just as the prototypical complex situation is spin-$\frac{1}{2}$ $\mathbf{J}\cdot\mathbf{B}$, the prototypical quaternionic situation is this spin-$\frac{3}{2}$ case.

Here are the main features of the spin-$\frac{3}{2}$ case.[5]

(a) The time-reversal–invariant traceless operators on $\mathbb{C}^4$ (equivalently traceless quaternionic Hermitian operators on $\mathbb{H}^2$) are exactly the family of $H(Q)$. This can be seen by just counting dimensions. Each is exactly five-dimensional and each $H(Q)$ is quaternionic, Hermitian, and traceless.

(b) Each nonzero $H(Q)$, being traceless, Hermitian, and 2×2 (quaternionically), can be written uniquely as

$$H=c(P_+-P_-)=c(2P_+-1)=c(1-2P_-),$$

where c is a positive real number and $P_\pm$ is the spectral projection onto the positive (or negative) eigenspace. Conversely, to each projection P and positive number c we can associate the Hamiltonian $c(2P-1)$. As a result, there is a one-to-one correspondence between the unit sphere of $H(Q)$'s and the set of spectral projections P_+ (or P_-), yielding the first proof that that the two

Chern integers are ± 1.

(c) $\mathrm{Tr}[H(Q)^2] = 6\mathrm{Tr}(Q^2)$. By (a), the unit sphere of $H(Q)$'s is left invariant by the full group of 2×2 symplectic matrices, $\mathrm{Sp}(2)\cong \mathrm{Spin}(5)$, the twofold universal cover of SO(5). Spin(5) acts on the unit sphere of Hamiltonians by SO(5) rotations. Thus, this family of operators, which *a priori* only has SO(3) symmetry, has SO(5) symmetry. Any Hamiltonian can be mapped to any other Hamiltonian by an SO(5) rotation, even though there are pairs of Hamiltonians that are not related by SO(3).

(d) Because all unit Hamiltonians are equivalent by the SO(5) symmetry, the second Chern form is a multiple of the area form. The constant of proportionality can be computed at any point [say $(J_z^2 - \frac{1}{3}J^2)$] to yield another proof that the two Chern integers are ± 1.

(e) Using the explicit matrices of J_x, J_y, and J_z in the spin-$\frac{3}{2}$ representation, one can easily check that the matrices e_α defined above form a Clifford algebra, i.e., $e_\alpha e_\beta + e_\beta e_\alpha = 2\delta_{\alpha\beta}$. The commutators $[e_\alpha, e_\beta]$ generate the Spin(5) action. By a unitary change of basis, these matrices can be transformed to

$$\hat{e}_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},\ \hat{e}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \hat{e}_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},$$

$$\hat{e}_3 = \begin{bmatrix} 0 & j \\ -j & 0 \end{bmatrix},\ \hat{e}_4 = \begin{bmatrix} 0 & -k \\ k & 0 \end{bmatrix},$$

which evidently span the traceless quaternionic Hermitian 2×2 matrices. The Clifford property makes the fact $P_\pm(Q) = \frac{1}{2}[1 \pm H(Q)]$ of (b) evident.

(f) For many paths on the four-sphere of Hamiltonians, the SO(5) symmetry enables one to compute the holonomy explicitly.[5] Specifically, consider paths of the form $H(\tau) = U(\tau)e_0 U(-\tau)$, $0 \le \tau \le 2\pi$, where $U(\tau)$ is a one-parameter group of symplectic matrices with $U(2\pi) = -1$. Paths of this form are closed, as $H(0) = H(2\pi) = e_0$. By (e), such one-parameter groups are of the form $U(\tau) = \exp(\tau C_{\alpha\beta}[e_\alpha, e_\beta])$ for appropriate constants $C_{\alpha\beta}$. In particular, the physical SO(3) rotations are of this type. Suppose the system is initially in an eigenstate of $J_z = m$. The probability of the final state being $J_z = -m$ is easily recovered from the holonomy, and is a physical observable amenable to experimental measurement. Consider a path generated by the physical rotation $U(\tau) = \exp\{-i\tau[\cos(\phi)J_z + \sin(\phi)J_x]\}$. For any path generated by physical rotation the probability of an initial state $J_z = \frac{3}{2}$ going to a final state $J_z = -\frac{3}{2}$ is zero. This result is based on an analysis of the geometry of SO(3) representations. The SO(3) symmetry further allows one to compute the probability of the $J_z = \frac{1}{2}$ state going to the $J_z = -\frac{1}{2}$, which is given by[6,13]

$$\frac{(4\sin^2\phi)\{\sin^2[\pi(1+3\sin^2\phi)^{1/2}]\}}{1+3\sin^2\phi}.$$

For paths which are generated by SO(5) rotations not corresponding to the physical rotations, the probability of $J_z = \frac{3}{2}$ going to $J_z = -\frac{3}{2}$ need not be zero. In fact, there exist paths for which this probability is unity, for example, the path generated by $U(\tau) = \exp[(\tau/8)e_1(\sqrt{3}e_0 + 2e_3)]$.

(g) This example is closely related to the symmetric SU(2) instanton.[14] The connection governing the adiabatic time evolution for the spin $\frac{3}{2}$ has self-dual curvature, and thus is a classical solution of the SU(2) Yang-Mills equations.

(h) Connections with self-dual curvature are classified via twistor theory,[14] and the spin-$\frac{3}{2}$ representation arises naturally in this framework. The rotation group SO(3) acts on the four-sphere of unit quadrupoles. The twistor space of S^4 is $\mathbb{C}P^3$, which now has an induced SO(3) action. This action extends to a projective representation of SO(3) on $\mathbb{C}^4$, which is precisely the spin-$\frac{3}{2}$ representation of SU(2).

The second Chern numbers may be thought of as quantum numbers that arise from topology rather than symmetry. Besides labeling the spectrum, quantum numbers that come from symmetry give various selection rules forbidding certain transitions. Similarly, the topological quantum numbers, besides labeling the spectrum give selection rules for adiabatic processes that can force transitions whenever the eigenstate bundle is nontrivial, at least for some paths. This holds on general grounds and is also illustrated by (f) above.

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[8]E. P. Wigner, Göttinger Nachr. **31**, 546 (1932). See also E. P. Wigner, *Group Theory* (Academic, New York, 1959). The connection between quaternions and antilinear operators with $T^2=-1$ and the fact that time-reversal invariance without reality has such a structure both have a long history in the mathematical literature on group representations. If U is an irreducible representation unitarily equivalent to its complex conjugate, then either U can be made simultaneously real or it is a quarternionic representation. Moreover, if the group is compact, which it is can be found by averaging the square of the group character over the group (this average is 1 in the real case and -1 in the quaternionic case). For finite groups, this result is called the Frobenius-Schur theorem, and goes back to the first decade of this century. In the terminology of modern representation theory, T is called a structure map. Applied to SU(2), it shows that the integral spin representations are real, while the half-odd-integral spin case is quaternionic.

[9]The unitary symplectic group Sp(n) (often called simply the symplectic group) consists of the $n\times n$ quaternion-valued matrices which preserve the usual norm on $\mathbb{H}^n$. The generators of Sp(n) are the Hermitian quaternionic matrices. If $\mathbb{H}^n$ is identified with $\mathbb{C}^{2n}$, Sp(n) is that subset of the complex unitary matrices U($2n$) which commute with T, and the quaternionic Hermitian matrices are those complex Hermitian matrices that commute with T. That $\mathrm{Sp}(1)\cong\mathrm{SU}(2)$, and $\mathrm{Sp}(2)\cong\mathrm{Spin}(5)$ is well known.

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