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LETTER TO THE EDITOR

Chern numbers for fermionic quadrupole systems

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Abstract. We analyse families of quantum quadrupole Hamiltonians $H = \Sigma_{\alpha\beta} Q_{\alpha\beta} J_\alpha J_\beta$ for half-odd-integer spin, and calculate the second Chern numbers of the energy levels. Each non-zero integer occurs only a finite number of times. The adiabatic time evolution, the non-Abelian generalisation of Berry's phase, is different for each system, in contrast to Berry's example. The $j=\frac{3}{2}$ and $j=\frac{1}{2}$ cases previously analysed are the only ones with self-dual curvatures and SO(5) symmetry.

Geometrical and topological techniques applied to the study of time-dependent quantum Hamiltonians have recently generated much interest [1]. Berry's examples of a family of Hamiltonians of the form $\boldsymbol{B} \cdot \boldsymbol{J}$ display the diversity of phenomena. The degenerate, or non-Abelian, case has received much attention [2]. In the class of time-reversal-invariant fermionic Hamiltonians, which have Kramers degeneracy [3], the quadrupole systems $\Sigma_{\alpha\beta} Q_{\alpha\beta} J_\alpha J_\beta$ for half-odd-integer spin are in many ways the analogues of Berry's examples [4]. The relevant topological invariants are the first Chern number over a 2-sphere for Berry's examples, and the second Chern number over a 4-sphere for the quadrupoles. Chern numbers are defined for energy levels which have a fixed degree of degeneracy for all Hamiltonians in the family. The Chern numbers for quadrupoles with $j \leq \frac{3}{2}$ are defined and have been previously computed [4].

In this paper, we will calculate the second Chern numbers for all quadrupole systems with half-odd-integer spin. In fact, every topological invariant of two-dimensional complex vector bundles over S^4 is a function of the second Chern number, i.e. these bundles are classified by the second Chern number up to topological equivalence. It will be shown in [5] that the second Chern numbers are indeed well defined for all half-odd-integer j.

An energy level can be specified by the eigenvalue of a particular Hamiltonian. It is convenient to take the quadrupole Hamiltonian $Q_0 = J_3^2 - \frac{1}{3}\boldsymbol{J}^2$ which commutes with J_3. The energy level can then be labelled by (j, m_{T}), where j is the total angular momentum and m_{T}^2 is the eigenvalue of J_3^2. We shall refer to this Hamiltonian as the north pole, and to minus this Hamilitonian as the south pole. The level can alternately be labelled by (j, m_{B}), where m_{B}^2 is the eigenvalue of J_3^2 at the south pole, with $m_{\mathrm{B}} = j + \frac{1}{2} - m_{\mathrm{T}}$.

Second Chern numbers over the 4-sphere will be calculated as the integral of the 4-form $\omega = -\mathrm{Tr}(\Omega \wedge \Omega)/8\pi^2$, where Ω is the curvature of the connection on the eigenstate bundle given by adiabatic time evolution [6]. As a first step we will reduce the integral of a general rotationally invariant 4-form over the 4-sphere of unit quadrupoles

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to a one-dimensional integral. We will then evaluate this integral for the Chern form, and determine the second Chern numbers to be $\frac{1}{2}(j+\frac{1}{2})(2m_T-j-\frac{1}{2})$. It follows that every non-zero integer appears as a Chern number a finite number of times, and zero appears an infinite number of times. All integers other than ± 1 and $\pm 2^k$, $k=1,2,3,\ldots,$ appear at least twice.

In Berry's example [1] two systems with the same Chern number have gauge-equivalent connections, because the connection with the required SU(2) symmetry is unique [7]. However, no two quadrupole systems have gauge-equivalent connections. That is, two systems with the same Chern number can be distinguished by their adiabatic time evolution properties. In the special case $j=\frac{3}{2}$ the connections have (anti) self-dual curvatures, and also have an SO(5) symmetry [4], properties which also hold trivially for $j=\frac{1}{2}$. However, neither of these properties ever occurs for $j>\frac{3}{2}$. These statements will be proven in [5].

We now begin by analysing the space of unit (normalised) quadrupoles, and the structure of the SO(3) orbits. There are exactly two two-dimensional orbits, and a one-parameter family of three-dimensional orbits. We express an integral of a rotationally invariant 4-form over the space of unit quadrupoles as an integral over this family.

A quadrupole Q is a 3×3 real symmetric matrix with zero trace. The space of quadrupoles is a five-dimensional real vector space, with an inner product $(Q, Q')=\frac{3}{2}\operatorname{Tr}(QQ')$. A unit quadrupole statisfies $\frac{3}{2}\operatorname{Tr} Q^2=1$. The space of unit quadrupoles is a 4-sphere.

The rotation group SO(3) acts on the space of quadrupoles by $Q\to RQR^{-1}$, preserving the inner product. The space of diagonal quadrupole matrices is two-dimensional, spanned by $Q_0=\operatorname{diag}(-\frac{1}{3},-\frac{1}{3},\frac{2}{3})$ and $Q_{\pi/2}=\operatorname{diag}(\sqrt{\frac{1}{3}},-\sqrt{\frac{1}{3}},0)$. Every symmetric matrix can be diagonalised by an orthogonal transformation, so every unit quadrupole is rotationally related to a diagonal unit quadrupole, i.e. a matrix of the form

$$Q_\theta=\cos(\theta)Q_0+\sin(\theta)Q_{\pi/2}=\tfrac{2}{3}\operatorname{diag}[\cos(\theta+2\pi/3),\cos(\theta-2\pi/3),\cos(\theta)]$$

for some value of $0\leq\theta<2\pi$.

In fact, every unit quadrupole is rotationally related to exactly one Q_θ with $0\leq\theta\leq\pi/3$, as we now show. The rotation $\exp[\pm\frac{2}{3}\pi\frac{1}{3}(L_1+L_2+L_3)]$ cyclically permutes the entries of Q_θ, so Q_θ is rotationally related to $Q_{(\theta\pm 2\pi/3)}$. Now the rotation $\exp(\frac{1}{2}\pi L_3)$ permutes the first two entries of Q_θ, so Q_θ is rotationally related to $Q_{-\theta}$. Thus any unit quadrupole is rotationally related to some Q_θ, with $0\leq\theta\leq\pi/3$. The θ in this interval is unique, because $\operatorname{Det}(Q_\theta)=\frac{2}{27}\cos(3\theta)$ is a one-to-one function on this interval. The south pole $-Q_0$ is rotationally related to $Q_{\pi/3}$, since $\operatorname{Det}(-Q_0)=\operatorname{Det}(Q_{\pi/3})$.

The orbits of Q_0 and $Q_{\pi/3}$ are two dimensional, while all the other orbits are three-dimensional. This is checked by noting that Q_0 and $Q_{\pi/3}$ each commute with exactly one generator of the rotation group, while Q_θ for $0<\theta<\pi/3$ does not commute with any of the generators. The subgroup $V\subset SO(3)$ which leaves Q_θ, $0<\theta<\pi/3$, invariant consists of four elements; $V=\{1,\exp(\pi L_1),\exp(\pi L_2,),\exp(\pi L_3)\}$. The assignment $R\to RQ_\theta R$ is thus four-to-one. Alternatively, we consider the double cover SU(2) of SO(3). Every Q_θ with $0<\theta<\pi/3$ is left invariant by the eight-element subgroup $F=\{\pm 1,\pm i\sigma_1,\pm i\sigma_2,\pm i\sigma_3\}$, which maps onto V under $SU(2)\to SO(3)$.

Denote by X the 4-sphere with the two-dimensional orbits removed. This is now an open four-dimensional manifold. The integral of a 4-form over S^4 is equal to the integral over X. There is a one-to-one correspondence between $Y\times I$ and X, where Y is the space $SU(2)/F$, and I is the interval $0<\theta<\pi/3$. We put coordinates on an open subset of X by

$$(y_1, y_2, y_3, \theta) \mapsto \exp(-iy_\alpha J_\alpha) Q_\theta \exp(iy_\alpha J_\alpha) \qquad \sum_\alpha (y_\alpha)^2 < \varepsilon \qquad 0 < \theta < \pi/3.$$

A rotationally invariant 4-form on X is constant on the orbits, and is uniquely determined by its value on one point of each orbit, e.g. on the set of points $I = (y_\alpha = 0, 0 < \theta < \pi/3)$. Every rotationally invariant 4-form ρ, expressed in local coordinates as

$$\rho = f(y_\alpha, \theta)\, d\theta \wedge dy_1 \wedge dy_2 \wedge dy_3 \tag{1}$$

is thus specified by the function $f(y_\alpha = 0, \theta)$. (Note that in these coordinates f is not constant along the orbits, because $dy_1 \wedge dy_2 \wedge dy_3$ is not the invariant measure on the orbit (see e.g. [8], exercise III.4.d, p 178).)

Integrating first over the orbits, we reduce the integral of a rotationally invariant 4-form ρ (expressed in local coordinates $\{y_\alpha, \theta\}$ as in (1)) over S^4 to a one-dimensional integral over a path connecting the two two-dimensional orbits:

$$\int_{S^4} \rho = 2\pi^2 \int_0^{\pi/3} f(\theta, 0)\, d\theta. \tag{2}$$

In fact, this equation is valid for an arbitrary path parametrised by θ that connects the two orbits. This follows from the invariance of the left-hand side under differentiable maps $S^4 \to S^4$ (of degree 1) which commute with rotations. Any path is the image of the standard path under some such map.

The normalisation constant $2\pi^2$ is the integral over any three-dimensional orbit of the invariant 3-form that equals $dy_1 \wedge dy_2 \wedge dy_3$ at the point $y_\alpha = 0$. SU(2) can be embedded as the unit sphere in R^4, since every SU(2) matrix can be uniquely written as $z_0 1 - iz_\alpha \sigma_\alpha$, with $z_0^2 + \Sigma_\alpha z_\alpha^2 = 1$. We can lift the coordinates $\{y_\alpha\}$ to coordinates on a neighbourhood of the identity in SU(2) by $\{y_\alpha\} \to \exp(-iy_\alpha \sigma_\alpha/2) = 1 - i\frac{1}{2}y_\alpha \sigma_\alpha + o(y^2)$. This has to lowest order the R^4 coordinates $z_0 = 1$, $z_\alpha = \frac{1}{2}y_\alpha$. So we find that $dy_1 \wedge dy_2 \wedge dy_3 = 8\eta$, where η is the three-dimensional area element on the unit sphere in R^4. Thus the integral over SU(2) is eight times the volume of the 3-sphere, or $16\pi^2$. Since SU(2) is an eightfold cover of each orbit, the integral over the orbit on X is one-eighth of this total, namely $2\pi^2$.

We now calculate the Chern numbers. We use the fact that the curvature Ω is rotationally invariant, as is the second Chern form $\omega_2 = -\mathrm{Tr}(\Omega \wedge \Omega)/8\pi^2$, which allows us to apply (2) to reduce the four-dimensional integral to a one-dimensional integral. The spectral projection $P(y_\alpha, \theta)$, and its derivative dP are given by

$$P(y_\alpha, \theta) = \exp(y_\alpha K_\alpha) P_\theta \exp(-y_\alpha K_\alpha)$$

$$dP(0, \theta) = [K_\alpha, P_\theta]\, dy_\alpha + P'\, d\theta$$

where the prime denotes a derivative with respect to θ. Here $K_\alpha = -iJ_\alpha$, in the appropriate representation of SU(2). From now on, all quantities are evaluated on the arc $y_\alpha = 0$, θ, and $P = P(0, \theta)$, etc. The curvature $\Omega = P dP \wedge dP P$ [9, 10] evaluated on the arc takes the form

$$\Omega = \sum_{\alpha<\beta} P[[K_\alpha, P], [K_\beta, P]]P\, dy_\alpha \wedge dy_\beta + \sum_\gamma P[[K_\gamma, P], P']P\, dy_\gamma \wedge d\theta.$$

Defining $V_\alpha = PK_\alpha P$, the second Chern 4-form $\omega_2 = -\mathrm{Tr}(\Omega \wedge \Omega)/8\pi^2$ equals

$$-\frac{1}{4\pi^2}\mathrm{Tr}\left(\sum_\alpha V_\alpha P V'_\alpha P - [V_1, V_2]PV'_3P - [V_2, V_3]PV'_1P - [V_3, V_1]PV'_2P\right)$$

$$= -\frac{1}{8\pi^2}\left[\mathrm{Tr}\left(\sum_\alpha V_\alpha V_\alpha - 2[V_1, V_2]V_3\right)\right]'$$

multiplied by $\mathrm{d}\theta \wedge \mathrm{d}y_1 \wedge \mathrm{d}y_2 \wedge \mathrm{d}y_3$. Now using (2), and the fact that $Q_{\pi/3}$ is rotationally related to $-Q_0$, we find

$$C_2 = -\frac{1}{8\pi^2}\int_{S_4} \mathrm{Tr}(\Omega \wedge \Omega) = g(-Q_0) - g(Q_0)$$

where the rotationally invariant function g is given by

$$g = \tfrac{1}{4}\left[\mathrm{Tr}\left(\sum_\alpha V_\alpha V_\alpha - 2[V_1, V_2]V_3\right)\right]$$

with $g(Q_0) = -\frac{1}{2}m_\mathrm{T}^2$, and $g(-Q_0) = -\frac{1}{2}m_\mathrm{B}^2$. This yields

$$C_2 = \tfrac{1}{2}(m_\mathrm{T}^2 - m_\mathrm{B}^2) = m_\mathrm{T}(j+\tfrac{1}{2}) - \tfrac{1}{2}(j+\tfrac{1}{2})^2$$

as shown in figure 1.

The set of Chern numbers is in one-to-one correspondence with the set $n(2k+1)$, with $n \in \mathbb{Z}$ and $k \in \mathbb{Z}_+$, the non-negative integers. This is easily seen pictorially, by following the lines in figure 1, and lets us calculate the number of times each integer l appears. Zero appears an infinite number of times. Assume l is positive, since l and $-l$ appear with the same frequency. l appears once for every distinct odd factor of l. For example, $90 = 1\times2\times3\times3\times5$; its odd factors are 1,3, 5, 9, 15, 45, so 90 appears six times. Clearly every number appears at least once, since every number has 1 as a factor. The number 1 and the powers of 2 appear exactly once. Odd primes larger than 1 appear exactly twice, as do products of odd primes with powers of two. All other numbers appear at least three times.

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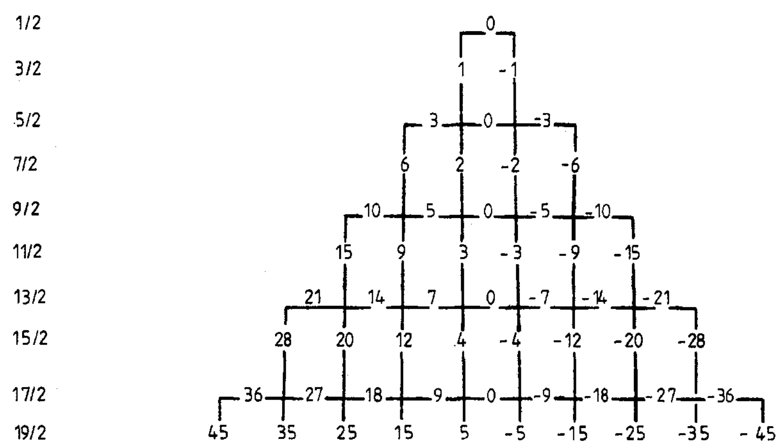

Figure 1. Chern numbers as a function of j. The numbers along each line are multiples of an odd integer. Each number appears as many times as it has distinct positive odd factors.

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