PHYSICAL REVIEW A

GENERAL PHYSICS

THIRD SERIES, VOLUME 38, NUMBER 1 JULY 1, 1988

Non-Abelian gauge structure in nuclear quadrupole resonance

A. Zee

Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

(Received 26 October 1987)

We elucidate the non-Abelian gauge structure associated with nuclear quadrupole resonance. The Abelian part of this structure has been experimentally observed. The phases to be observed in various non-Abelian experiments are computed.

Berry's remarkable discovery[1,2] that gauge structures exist naturally in slowly varying quantum systems has generated a great deal of interest,[3-9] both theoretically and experimentally. In particular, it has been shown[4] that a non-Abelian gauge structure emerges if a set of quantum states remains degenerate as the Hamiltonian varies.

In an interesting recent experiment, Tycko[9] demonstrated the effect of Berry's phase on the magnetic resonance spectrum of a rotating magnetic sample by using a pure nuclear quadrupole resonance. The spin quadrupole Hamiltonian describing Tycko's experiment is effectively given by

$$H=(\mathbf{S}\cdot\mathbf{B})^2$$

$$=(S_x\sin\theta\cos\varphi+S_y\sin\theta\sin\varphi+S_z\cos\theta)^2B^2\ . \quad (1)$$

Besides being invariant under rotation and under time reversal ($\mathbf{S}\rightarrow-\mathbf{S}$ and $\mathbf{B}\rightarrow-\mathbf{B}$), the Hamiltonian is also invariant under the operation $\mathbf{S}\rightarrow-\mathbf{S}$. It is of course this additional symmetry (of the instantaneous Hamiltonian) that guarantees the pairwise degeneracy of states as we move about in parameter space (that is, as we vary $\mathbf{B}$ adiabatically).

In the actual experiment, a spin-$\frac{3}{2}$ Cl atom in a $NaClO_3$ crystal is used. Clearly, the four spin-$\frac{3}{2}$ states fall into two doubly degenerate sets and thus we can expect to see a non-Abelian gauge structure in accordance with the general analysis of Ref. 4. Unfortunately, the actual experimental setup was such that only Abelian phases were observed. In Tycko's experiment, the magnetic field results from an internal electric field gradient in the crystal. When the crystal is rotated, an effective magnetic field arises. In the subsequent theoretical analysis, we will just treat the equivalent problem of a spin in a rotating magnetic field and we will speak as if an external magnetic field were being rotated. In this paper, we elucidate the non-Abelian structure and comment on how this structure can be observed in experiments analogous to (but more complicated than) Tycko's.

We begin by reviewing the general framework. Let η_a be an N-fold degenerate set of orthonormal instantaneous eigenstates of the Hamiltonian $H\mid\eta_a\rangle=E\mid\eta_a\rangle$. (With no loss of generality, by replacing H by $H-E$, we can set $E=0$.) The assumption that H varies adiabatically implies that the true wave function may be expanded in terms of $\mid\eta_a\rangle$: $\mid\psi_a\rangle=\sum_b\mid\eta_b\rangle U_{ba}$. Plugging into $i(\partial/\partial t)\mid\psi_a\rangle=H\mid\psi_a\rangle$, we find immediately that

$$\dot{U}_{ba}=-\sum_c\langle\eta_b\mid\dot{\eta}_c\rangle U_{ca}\ . \quad (2)$$

Berry's essential insight was the recognition, in the nondegenerate case, that the phase $\langle\eta\mid\dot{\eta}\rangle$ cannot be trivially absorbed, as was erroneously asserted by various standard texts read by generations of physicists. Rather, a gauge structure can be defined as follows. In general, H depends on a number of parameters $x^\mu,\mu=1,\ldots,p$, and H varies as the parameters $x^\mu(t)$ vary with time. We can thus define the gauge potential

$$A_{ab\mu}=\left\langle\eta_a\left|\frac{\partial}{\partial x^\mu}\right|\eta_b\right\rangle\ , \quad (3)$$

so that $\langle\eta_a\mid\dot{\eta}_b\rangle=\sum_\mu A_{ab\mu}(dx^\mu/dt)$ and Eq. (2) can be integrated immediately to give

$$U_{ab}=\left[\mathcal{P}\exp\left[-\int A_\mu dx^\mu\right]\right]_{ab}\ , \quad (4)$$

where $\mathcal{P}$ indicates to path-ordered product. In what follows, we use the notation of differential forms and write $A_{ab}=A_{ab\mu}dx^\mu$. We will also suppress the indices $a,b,\ldots$, on the matrix form. The gauge group in question corresponds to the unitary freedom in choosing the basis states $\mid\eta_a\rangle$. With a different choice $\mid\eta'_a=\sum_b\mid\eta_b\rangle\omega_{ba}$, we have the transformed gauge potential $A'=\omega^\dagger A\omega+\omega^\dagger d\omega$. Here ω is an $N\times N$ unitary matrix. The gauge field $F=dA+A\wedge A$ transforms covariantly, of course: $F'=\omega^\dagger F\omega$. The trace of U for a closed loop is gauge invariant. Thus we have a

$U(N)=SU(N)\times U(1)$ gauge field existing on a p-dimensional space.

After a complete cycle, the physical situation returns to what it was at the start of the cycle but the states $|\eta_a\rangle$ are multiplied by the unitary matrix $U=\mathcal{P}\exp(-\oint A)$. The states evolve into linear combinations of each other. Diagonalizing U to have eigenvalues e^{iE_iT} (where T is the time taken to complete the cycle), we can also say that the corresponding eigenstate has shifted in energy by E_i.[10] The unitarity of U implies that $\sum_i E_i T$ is an integer multiple of 2π (see below).

Given this general framework, we can easily calculate the gauge potential by parametrizing the Hamiltonian in Eq. (1) as

$$H=B^2e^{-i\varphi S_z}e^{-i\theta S_y}S_z^2e^{i\theta S_y}e^{i\varphi S_z}, \tag{5}$$

keeping in mind that this set of coordinates is not everywhere defined on the 2-sphere. (This fact introduces certain subtleties to be discussed below.) Then, as noted in Ref. 4, we obtain the instantaneous eigenstates immediately as

$$|\eta_a\rangle=e^{-i\varphi S_z}e^{-i\theta S_y}|a\rangle,$$

where $|a\rangle$, $|b\rangle$, and so on, are simply (1,0,0,0) etc., in the standard spinor notation. We proceed with the calculation taking the spin S as arbitrary. [Notice as usual that for S half-integral $|\eta_a\rangle$ at $\varphi=2\pi$ is equal to (-1) times $|\eta_a\rangle$ at $\varphi=0$. The states $|\eta_a\rangle$ provide a double covering of parameter space. Thus, the phase factor U determines the phase change in addition to the phase produced by rotation through 2π.] Evaluating the general formulas (3), we find

$$\begin{aligned} A_{ab\varphi}&=(-i)\langle a|(\cos\theta S_z-\sin\theta S_x)|b\rangle, \\ A_{ab\theta}&=(-i)\langle a|S_y|b\rangle. \end{aligned} \tag{6}$$

It is worth emphasizing that these formulas are quite general and hold whenever H has the form

$$H=e^{-i\varphi S_z}e^{-i\theta S_y}H_0e^{i\theta S_y}e^{i\varphi S_z}.$$

The "unrotated" Hamiltonian H_0 serves only to determine the degeneracy structure, namely, the gauge group. In particular, it does not matter if H_0 is S_z^2 or S_z raised to any even power. Also, H_0 can in general be a many-body Hamiltonian. The analysis also clearly does not depend on the system being nuclear. We also remark that if H_0 is anisotropic, for instance, $H_0=\alpha S_x^2+\beta S_y^2+\gamma S_z^2=\alpha' S_x^2+\gamma' S_z^2+\text{const}$, we will have to use the general rotation $e^{i\psi S_z}e^{i\theta S_y}e^{i\varphi S_z}$ and the gauge potential will exist on a three-dimensional space.

The states $|a\rangle$ can be taken to be the eigenstates $|m\rangle$ with $S_z|m\rangle=m|m\rangle$. For the problem at hand, the states $(\pm m)$ form a doubly degenerate secotr. For $|m|\neq\frac{1}{2}$, we obtain only an Abelian structure with $A_\theta=0$ and $A_\varphi=(-i)m\cos\theta$. This follows since $\mathbf{S}$ cannot cause transition with $\Delta m>1$. The corresponding field strength $F=(-i)m\,d\Omega$ (where $d\Omega=\sin\theta\,d\theta\,d\varphi$ is the invariant area element) shows that the gauge potential is that which is generated by a monopole of strength $2m$.

It may be instructive to compare the nondegenerate situation studied by Berry,[1] namely, that for the spin dipole Hamiltonian $H=\mathbf{S}\cdot\mathbf{B}$. As remarked above, the "unrotated" Hamiltonian H_0, here BS_z, serves only to determine the degeneracy structure. Thus, the formulas in (6) apply, with the indices a and b and A omitted and with the states $|a\rangle$ comprised of some eigenstates of S_z with eigenvalue m. Berry thus obtained $A_\theta=0$ and $A_\varphi=(-i)m\cos\theta$ exactly as in the preceding, except that m may be equal to $\frac{1}{2}$ in this case.

In the $|m|=\frac{1}{2}$ sector we obtain a truly non-Abelian structure with

$$A=(-i)\left[\left(\cos\theta\frac{\sigma_3}{2}-\alpha\sin\theta\frac{\sigma_1}{2}\right)d\varphi+\alpha\frac{\sigma_2}{2}d\theta\right], \tag{7}$$

with $\alpha\equiv S+\frac{1}{2}$ an integer. In this sector, while S_z is represented by $\sigma_3/2$, S_x and S_y are represented by $\alpha(\sigma_1/2)$ and $\alpha(\sigma_2/2)$, respectively. The corresponding gauge field

$$F=(-i)(\alpha^2-1)\frac{\sigma_3}{2}d\Omega$$

is formally the same as the Abelian field strength in the $|m|\neq\frac{1}{2}$ sector. Nevertheless, the gauge structure is non-Abelian. What is physically relevant is not so much F as the Wilson loop

$$\mathrm{Tr}U=\mathrm{Tr}\mathcal{P}\exp\left[-\oint A\right];$$

the path ordering is clearly essential. Note that the gauge field does not satisfy the sourceless Yang-Mills equation. In particular, $F_{\theta\varphi}$ does not depend on φ, while $[A_\varphi,F_{\theta\varphi}]$ is proportional to $\sin^2\theta\sigma_2$. Note also that F vanishes for $\alpha=1$ (that is, $S=\frac{1}{2}$) as it should since the problem collapses in that case, H_0 (and therefore H) being proportional to the unit matrix.

We now see that, since in Tycko's experiment θ is held fixed (with $\cos\theta=1/\sqrt{3}$) while φ varies cyclically, the non-Abelian character of A is lost. (The reason that the fixed θ path is followed in Tycko's experiment is simply that a rotation about a fixed axis is the only rotation of a crystal that can be performed rapidly enough to produce an observable phase shift.) A is proportional to the fixed matrix $(\cos\theta\sigma_3-\alpha\sin\theta\sigma_1)$ with eigenvalues $\pm(\cos^2\theta+\alpha^2\sin^2\theta)^{1/2}$ and thus after each rotation of φ through 2π we obtain the phase shifts $\pm\pi(\cos^2+\alpha^2\sin^2\theta)^{1/2}$ for the appropriate eigenstates, in agreement with Tycko for $\alpha=2$ (that is, $S=\frac{3}{2}$). As the magnetic field turns, the two states $|\eta_{+(1/2)}\rangle$ and $|\eta_{-(1/2)}\rangle$ rotate into a linear combination of each other. The two degenerate levels are split by $\Delta E=2\pi(\cos^2\theta+\alpha^2\sin^2\theta)^{1/2}/T$, where T is the time period over which the adiabatic variation goes through one cycle. Note that at $\theta=\pi/2$ the phase factor $e^{\pm i\pi\alpha}$ acquired in each cycle is $+1$ or -1 for $\alpha=S+\frac{1}{2}$ even or odd, respectively. Actually, there is an additional

factor of (-1) to be explained later. [Also note that the $+$ eigenstate is largely the spin up state near the north pole ($\theta\sim 0$) and turns into the spin down state near the south pole ($\theta\sim\pi$). The same applies for the $-$ eigenstate.]

(There is a point of potential confusion here. It would appear naively that even in the $\alpha=1$ case the two states are split by $2\pi/T$, while, in fact, the Hamiltonian is proportional to the identity operator. The resolution is, of course, that when a quantum state has acquired a phase $e^{i\xi}$ it is the phase factor $e^{i\xi}$ and not the phase angle ξ that is defined. Thus $e^{i\pi}$ and $e^{-i\pi}$ represent the same phase. In other words, by looking at Berry's phase, the energy splitting is determined as only modulo $2\pi/T$. Note that this ambiguity is of the same order in $1/T$ as the energy splitting and so is potentially substantive. In Tycko's experiment, however, the ambiguity can be resolved, since we can follow the buildup of Berry's phase infinitesimally in time. With the fixed-θ path chosen by Tycko, the derivative of Berry's phase with respect to φ is a constant: A does not depend on φ. In other words, the physical situation in Tycko's experiment is essentially stationary. Thus we can integrate the phase change to obtain the phase shifts per cycle as cited above.)

In this gauge, the state $|m=+\frac{1}{2}\rangle$ is rotated by the matrix $\exp i\pi(\cos\theta\sigma_3-\alpha\sin\theta\sigma_1)$ into a linear combination of itself and the state $|m=-\frac{1}{2}\rangle$. It is easy enough to go to another gauge by diagonalizing the matrix

$$(\cos\theta\sigma_3-\alpha\sin\theta\sigma_1)=\omega\cos\theta\sigma_3\omega^{\dagger}$$

with $\omega=e^{i\chi(\sigma_2/2)}$ and $\tan\chi=\alpha\tan\theta$, that is, instead of the basic states $|\eta_a\rangle$ we choose $|\eta_a'\rangle=\sum_b|\eta_b\rangle\omega_{ba}$. Thus we compute

$$A'=\omega^{\dagger}A\omega+\omega^{\dagger}d\omega$$
$$=(-i)\left[\frac{\cos\theta}{\cos\chi}\frac{\sigma_3}{2}d\varphi+\frac{(\alpha^2-1)}{\alpha}\sin^2\chi\frac{\sigma_2}{2}d\theta\right]. \quad (8)$$

In this basis,

$$F'=(-i)(\alpha^2-1)\left[\cos\chi\frac{\sigma_3}{2}+\sin\chi\frac{\sigma_1}{2}\right]d\Omega .$$

Note that $\cos\theta/\cos\chi=(\cos^2\theta+\alpha^2\sin^2\theta)^{1/2}$ as it should.

To observe the non-Abelian character of Berry's phase in this situation, it is necessary to vary θ as well as φ. In general, we would like to compute U for an arbitrary loop on the 2-sphere. In practice, the computation is intrinsically non-Abelian and difficult, since each segment in the time-ordered exponential loop integral does not commute with the next. The integral can, however, be evaluated by numerical methods.

At first sight, one might think that one could compute U for loops consisting of cyclic motion on the sphere, maintaining a fixed angle with some arbitrary unit vector. It would appear that the non-Abelian structure would come into play, since both θ and φ vary. However, it is clear that the original Hamiltonian is rotational invariant and the z axis is preferentially picked out only by convention. The gauge factor obtained can only differ from the gauge factor obtained by tracing the "standard" fixed-θ loop (with the appropriate θ) by an inessential similarity transformation. This rotational invariance is reflected in the invariance of gauge invariant (geometrical) quantities such as

$$\mathrm{Tr}F\wedge *F=(-)(\alpha^2-1)^2\tfrac{1}{2}\sin\theta\,d\theta\,d\varphi .$$

Under a rotation, the gauge potential A changes by a gauge transformation, of course.

We note that the gauge potential we obtain here is the same as the gauge potential obtained by Wilczek *et al.*[5] in an analysis of diatomic molecules. This is hardly surprising: although the physical situations involved are different, the mathematical steps leading to the determination of the gauge potential are the same. In more mathematical language, one would say that the rotationally invariant connection on the sphere is essentially unique. A general (but rather involved) proof has been given by Forgacs and Manton.[11] A casual proof acceptable to many physicists can be sketched as follows. Let $F=\sum_j C_j(\sigma_j/2)d\Omega$. Since

$$\mathrm{Tr}F\wedge *F=\left[\sum_j C_j\right]^2\tfrac{1}{2}d\Omega ,$$

$\sum_j C_j^2$ is invariant by assumption. By a gauge transformation, we can rotate C_j to the standard form $C_1=C_2=0$ and $C_3=\text{const}$. The loophole is, of course, the question of whether the required gauge transformation can be carried out globally.

As noted, to explore the non-Abelian structure in nuclear quadrupole resonance, we should traverse a "non-Abelian" path in which θ and φ both vary. It seems to us that such a path can be traced in an experiment with an external magnetic field by varying the field suitably. For instance, we may have crossed magnetic fields with B_z varying at a different frequency from B_x and B_y. Of course, we also do not want T to be so large that the energy splitting is infinitesimal.

To "see" the non-Abelian character of the gauge structure, we have to show how the noncommutativity produces physically observable effects. Consider three closed loops A, B, and C, that all start (and end) at the same point x_0 on the sphere. Denote the phase factor generated by traversing each of the three loops to be U_A, U_B, and U_C, respectively. Consider the composite path in which one traverses first A, then B, and finally C. After a cycle, the phase factor $U=U_CU_BU_A$ is generated. In contrast, were one to traverse the three loops in the order, first A, then C, then B, the phase factor would be $U'=U_BU_CU_A$. while $\det U=\det U'$, in general $\mathrm{Tr}U$ is not equal to $\mathrm{Tr}U'$ and thus U and U' have different eigenvalues leading to different energy shifts.[12] Of course, each of the loops A, B, and C may be traversed many times, in which case U_A, U_B, and U_C represent the phase factor for each loop raised to a suitable power.

We were told[13] that in certain types of experiments it may be easiest to trace paths made up of segments along which either θ or φ is fixed. (It is not clear to us, however, how to go around the "corners.") Theoretically, it is of course effortless to calculate U for such path segments.

We now mention some subtleties associated with the

usual difficulty with spherical coordinates, namely, that φ is not defined at the north and south poles. To see that something is remiss, consider computing

$$U=\mathcal{P}\exp\left[-\int A\right]$$

for an infinitesimal small loop circling the north pole. We find, using (7), that $U\sim e^{i(\sigma_3/2)2\pi}=(-1)$. Thus there is a singularity at the north pole. Similarly, there is a singularity at the south pole. The gauge potential in (7), call it A_E (E for equatorial), can only be defined on a coordinate patch including the equator but excluding the north and south poles.

To understand what is going on, we refer to the analogous situation of the Dirac monopole. As noted earlier, the same formulas that produce A_E also produce in the Abelian case the gauge potential $a_E=(-i)m\cos\theta\, d\varphi$ and the gauge field $f_E=da_E=(-i)m\, d\Omega$. Here too, the phase factor $\exp(-\int a_E)$ for an infinitesimal small loop circling the north pole is equal to $\sim e^{im2\pi}=(-1)$ for $m=\frac{1}{2}$. Similarly, there is a singularity at the south pole. Consider, in contrast, the gauge potential $a_S=(-i)m(1+\cos\theta)d\varphi$. Clearly, since a_S and a_E differs only by a term proportional to $d\varphi$, the corresponding gauge field f_S is identical to f_E. The same remark can be made for the gauge potential $a_N=(-i)m(-1+\cos\theta)d\varphi$. Suppose for the moment that m is not known. Since $(1+\cos\theta)$ vanishes at the north pole, a_S is defined on the sphere excluding a region around the north pole. Similarly, a_N is defined on the sphere excluding a region around the south pole. The requirement is that in the overlap region where both a_N and a_S are defined they must be related by a gauge transformation. We have $a_N-a_S=2imd\varphi=e^{-2im\varphi}de^{2im\varphi}$. Indeed, a_N and a_S are related by a gauge transformation effected by $e^{2im\varphi}$, provided that $e^{2im\varphi}$ is defined, that is, if $e^{2im(2\pi)}=1$. Thus m is quantized to be integer multiple of $\frac{1}{2}$. This represents one of the standard arguments[14] for the quantization of magnetic charge.

But what about a_E? Since $a_N-a_E=imd\varphi=e^{-im\varphi}de^{im\varphi}$, a_E is related to a_N by a gauge transformation effected by $e^{im\varphi}$. However, for m half-integral, this gauge transformation, although locally legitimate, is not globally legitimate. The phase integral $\exp(-\int a_E)$ integrated from $\varphi=0$ to 2π differs from $\exp(-\int a_N)$ by $e^{im2\pi}=(-1)$ for m half-integral.[15] One way of describing the situation is that the equatorial patch on which a_E is defined is not a legitimate patch since it is not simply connected. (Strictly speaking, the patches on which a_N and a_S are located should be subdivided into smaller patches. The overlaps between patches are also required to be patches and hence each of the overlaps has to be simply connected.)

It is now clear what the problem is with the non-Abelian gauge potential A_E. By analogy with the Abelian case, we can define $A_S=\rho^\dagger A_E\rho+\rho^\dagger d\rho$ with the globally illegitimate (but locally legitimate) gauge transformation with $\rho=e^{-i(\sigma_3/2)\varphi}$. We obtain

$$A_S=(-i)\left\{\left[(1+\cos\theta)\frac{\sigma_3}{2}-\alpha\sin\theta\left(\cos\varphi\frac{\sigma_1}{2}-\sin\varphi\frac{\sigma_2}{2}\right)\right]d\varphi+\alpha\left(\cos\varphi\frac{\sigma_2}{2}+\sin\varphi\frac{\sigma_1}{2}\right)d\theta\right\}. \tag{9}$$

The result is more complicated in the non-Abelian case but the essential feature is that the combination $(1+\cos\theta)$ ensures that A_S is not singular at the south pole. We can now also define $A_N=\rho^2A_S\rho^{2\dagger}+\rho^2d\rho^{2\dagger}$ with a globally legitimate gauge transformation with the single-valued function $\rho^2=e^{-i\sigma_3\varphi}$. For completeness, let us record that

$$A_N=(-i)\left\{\left[(-1+\cos\theta)\frac{\sigma_3}{2}-\alpha\sin\theta\left(\cos\varphi\frac{\sigma_1}{2}+\sin\varphi\frac{\sigma_2}{2}\right)\right]d\varphi+\alpha\left(\cos\varphi\frac{\sigma_2}{2}-\sin\varphi\frac{\sigma_1}{2}\right)d\theta\right\}. \tag{10}$$

The moral of the story is that we should use A_N and A_S rather than A_E. However, we note that in practice it is easier to compute with A_E. For instance, along a fixed θ path, A_N and A_S depend on φ, while A_E does not. We can always use A_E, keeping in mind that for a line segment from point 1 to point 2

$$\exp\left[-\int_1^2 A_E\right]=\rho(2)\exp\left[-\int_1^2 A_S\right]\rho^\dagger(1).$$

Thus, for a closed path over whith φ does not vary by more than 2π, $\mathrm{Tr}U$ can be safely computed with A_E. On the other hand, for a path that wraps around once from $\varphi=0$ to $\varphi=2\pi$, $\exp(-\oint A_E)$ differs from $\exp(-\oint A_S)$ [and $\exp(-\oint A_N)$] by an extra factor of $e^{-i\sigma_3\pi}=(-1)$. This factor, however, does not matter in the computation of energy splitting. Thus, in particular, contrary to what was stated earlier, the phase factor acquired in each cycle around the equator should actually be (-1) or $(+1)$ for $\alpha=$ even or odd, respectively.

The careful discussion above is necessary; otherwise, one can easily fall into confusing traps. For instance, it is contemplated experimentally[13] to have a path (the "orange slice") going from the north pole to the south pole along some longitude and then back to the north pole along some other longitude. By looking at A_E [in Eq. (7)] one would conclude erroneously that since the gauge potential is independent of φ the phase acquired on the south-bound leg cancels that acquired on the north-bound leg and the net phase factor is unity. To do the calculation correctly, we must compute with A_N (say) and take care to stay within the north patch. We will actually compute the phase factor for the "spherical triangle" path in which we start from the north pole and go south at a fixed φ_1 to latitude θ, go at fixed θ to φ_2, and

then return to the north pole along longitude φ_2. The phase factor desired for the "orange slice" path is then obtained in the limit $\theta \to \pi$.

Since the final quantity $\mathrm{Tr}U_{\mathrm{ST}} = \mathrm{Tr}\exp(-\int_{ST} A_N)$ (ST stands for spherical triangle) can only depend on $\varphi_2 - \varphi_1$, we take $\varphi_1 = 0$ and $\varphi_2 = \Delta$. We read off from Eq. (10) that we have for the south-bound leg $W = e^{i\alpha(\sigma_2/2)\theta}$ and for the north-bound leg

$$(W')^{-1} = \exp\left[-i\alpha\frac{\theta}{2}(\cos\Delta\sigma_2 - sim\,\Delta\sigma_1)\right] .$$

For the east-bound leg along fixed θ, we note that A_N varies along the integration path. Fortunately, we know that

$$\begin{aligned} V &= \exp\left[-\int_1^2 A_N\right] \\ &= \rho_2 \exp\left[-\int_1^2 A_E\right]\rho_1^{\dagger} \\ &= \exp - i\sigma_3\Delta/2 \exp[i(\cos\theta\sigma_3 - \alpha\sin\theta\sigma_1)\Delta/2] . \end{aligned} \tag{11}$$

We are thus to evaluate $\cos\gamma_{\mathrm{ST}} = \frac{1}{2}\mathrm{Tr}U_{\mathrm{ST}} = \frac{1}{2}\mathrm{Tr}(W')^{-1}VW$. (This implies an energy splitting of $\Delta E = 2\gamma/T$, of course.) After a tedious computation, we find

$$\cos\gamma_{\mathrm{ST}} = \cos\eta\cos\frac{\Delta}{2} + \sin\eta\sin\frac{\Delta}{2}\cos(\chi - \alpha\theta) , \tag{12}$$

where $\eta = (\cos^2\theta + \alpha^2\sin^2\theta)^{1/2}\Delta/2$ and χ is as defined earlier.

Let us look at some special cases of this otherwise rather opaque expression. As $\theta \to \pi$, we have for the "orange slice" path

$$\cos\gamma_{\mathrm{OS}} = \cos^2\frac{\Delta}{2} - (-1)^{\alpha}\sin^2\frac{\Delta}{2} . \tag{13}$$

This is decidedly not unity as one would conclude erroneously from computing with A_E naively. In particular, for $\Delta = \pi$, we have the factor $(-1)^{\alpha+1}$. [This factor can of course also be read off directly with $W = (W')^{-1} = e^{i\alpha\sigma_2\pi/2}$ and $V = e^{-i\sigma_3\pi} = (-1)$.] Note that since the path is a great circle this factor must agree with the phase acquired upon going around the equator once as computed from Eq. (7) but with an extra factor of (-1) included.

For $\theta = \pi/2$, we have $\eta = \alpha\Delta/2$ and $\chi = \pi/2$, and thus

$$\cos\gamma^{o}_{\mathrm{ST}} = \cos\frac{\alpha\Delta}{2}\cos\frac{\Delta}{2} + \sin\frac{\alpha\Delta}{2}\sin\frac{\Delta}{2}\sin\frac{\alpha\pi}{2} . \tag{14}$$

For α even, this is equal to $\cos\alpha\Delta/2\cos\Delta/2$, for α odd of the form $4k+1$ with k an integer, $\cos(\alpha-1)\Delta/2$, and for α odd of the form $4k+3$, $\cos(\alpha-1)\Delta/2$. Perhaps this peculiar dependence on α can be tested by using nuclei with different spin.

In practice, it is easier to compute with A_E [or its gauge transform in Eq. (8)] than with A_N and A_S. As long as the path under consideration does not touch the poles and does not wrap around the sphere, we can safely compute with A_E. For instance, we can compute the phase factor U_{SR} obtained for the "spherical rectangle" path starting from the point (θ_1,ϕ_1), then going to (θ_2,ϕ_1) along a fixed-ϕ path, then to (θ_2,ϕ_2) along a fixed-θ path, then to (θ_1,ϕ_2) along a fixed-ϕ path, and finally back to (θ_1,ϕ_1) along a fixed-θ path. We find readily that

$$\tfrac{1}{2}\mathrm{Tr}U_{\mathrm{SR}} = \cos\frac{p_1\Delta}{2}\cos\frac{p_2\Delta}{2} + \sin\frac{p_1\Delta}{2}\sin\frac{p_2\Delta}{2}\cos Q , \tag{15}$$

where $p_i = (\cos^2\theta_i + \alpha^2\sin^2\theta_i)^{1/2}$, $Q = \alpha(\theta_2 - \theta_1) - (\chi_2 - \chi_1)$, and $\Delta = \phi_2 - \phi_1$. As $\theta_1 \to 0$, this expression reduces to the result for "spherical triangle," Eq. (12).

Incidentally, we can now read off the rotation of states in Tycko's experiment. The appropriate phase factor as the magnetic field is moved along a fixed-θ path from $\phi = 0$ to $\phi = \Delta$ is given by V in Eq. (11). In particular, starting with the initial state $|\eta_+\rangle = (1,0)$, we find the amplitude of being in the state $|\eta_-\rangle = (0,1)$ to be $(-i)\sin\eta\sin\chi e^{i\Delta/2}$, which we note vanishes only for some certain values of Δ, namely, for

$$\Delta = 2k\pi/(\cos^2\theta + \alpha^2\sin^2\theta)^{1/2}, \quad k = \text{integer} . \tag{16}$$

As already mentioned, V contains an extra factor of $e^{-i\sigma_3\pi} = (-1)$ for $\Delta = 2\pi$.

In the Abelian situation,[1] Berry could, and wisely did, avoid these complications by immediately using Stokes's theorem to write all expressions in terms of the gauge field F. The corresponding theorem is, however, not available for non-Abelian gauge potentials.

Incidentally, our discussion also allows us to illustrate an interesting feature of non-Abelian gauge potentials. Suppose we are given the gauge field

$$F = (-i)(\alpha^2 - 1)\frac{\sigma_3}{2}d\Omega$$

on the sphere. We know that the field strengths F_N, F_S, and F_E calculated from A_N, A_S, and A_E, respectively are all equal to $F_N = F_S = F_E = F$, since these three gauge potentials are related by (locally legitimate) gauge transformations that commute with σ_3. (We can of course also check this equality by direct computation.) However, as already noted, $\mathrm{Tr}\mathcal{P}\exp(-\int A_E)$ differs by a factor of (-1) from $\mathrm{Tr}\mathcal{P}\exp(-\int A_{N,S})$. This represents a non-Abelian version of the Aharonov-Bohm phenomenon. Imagine removing the caps around the north and south poles. Knowing the field strength in the nonsimply corrected equatorial "patch" does not determine for us the net phase change as we go around the loop.

Consider next the gauge potential

$$A_X = (-i)(\alpha^2 - 1)\cos\theta\frac{\sigma_3}{2}d\phi$$

with the corresponding field strength $F_X = F_N = F_S = F_E = F$. As we go around the equator once,

$$\mathrm{Tr}\exp\left[-\int A_X\right] = \mathrm{Tr}\exp[i(\alpha^2 - 1)\pi\sigma_3] .$$

Since this differs from $\mathrm{Tr}\exp(-\int A_E)=\mathrm{Tr}\exp(i\alpha\pi\sigma_3)$, A_X is clearly not related to A_E by a globally legitimate gauge transformation. In fact, A_X is not even related to A_E by a locally legitimate gauge transformation. To see this, we consider the gauge covariant quantity $D_\phi F_{\theta\phi}=\partial_\phi F_{\theta\phi}+[A_\phi,F_{\theta\phi}]$, namely, the source current of the gauge field. Computed with A_X, this quantity is clearly zero. On the other hand, as has already been noted, it is not zero when computed with A_E. This is in contrast to the Aharonov-Bohm phenomenon, in which the two relevant gauge potentials, while not related by a globally legitimate gauge transformation, are related by a locally legitimate gauge transformation.[16]

In their original discussion on non-Abelian gauge structures, Yang and Mills spoke of the degeneracy of the proton and neutron under isospin and imagined transporting a proton from one point in the universe to another. That a proton at one point can be interpreted as a neutron at another in an isospin invariant world necessitates the introduction of a non-Abelian gauge potential. We find it amusing that this discussion can now be realized analogously in the laboratory.

We are grateful to Y. S. Wu for helpful discussions. We would also like to thank M. Goodman and A. Strominger for useful conversations and F. Wilczek for encouraging us to publish this paper. We have also benefited from conversations with A. Pines and R. Tycko. This research was supported in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration, at the University of California at Santa Barbara.

---

[1]M. V. Berry, Proc. Roy. Soc. London, Ser. A **392**, 45 (1984). For a review and further references, see R. Jackiw, Massachusetts Institude of Technology. Report No. MIT-CTP-1475, 1987 (unpublished).

[2]G. Herzberg and H. C. Longuet-Higgins, Discuss. Faraday Soc. **55**, 77 (1963); C. A. Mead, Chem. Phys. **49**, 23 (1980); C. A. Mead and D. G. Truhlar, J. Chem. Phys. **70**, 2284 (1979); R. L. Whetten, G. S. Ezra, and E. R. Grant, Ann. Rev. Phys. Chem. **36**, 277 (1985).

[3]B. Simon, Phys. Rev. Lett. **51**, 2167 (1983); J. E. Avron, R. Seiler, and L. G. Yaffe, Commun. Math. Phys. **110**, 33 (1987).

[4]F. Wilczek and A. Zee, Phys. Rev. Lett. **52**, 2111 (1984).

[5]J. Moody, A. Shapere, and F. Wilczek, Phys. Rev. Lett. **56**, 893 (1986).

[6]H. Kuratsuji and S. Iida, Phys. Rev. Lett. **56**, 1003 (1986).

[7]R. Y. Chiao and Y. S. Wu, Phys. Rev. Lett. **57**, 933 (1986); A. Tomita and R. Y. Chiao, *ibid.* **57**, 937 (1986); M. V. Berry, Nature **19**, 277 (1987).

[8]Y. Aharonov and J. Anandan, Phys. Rev. Lett. **58**, 1593 (1987).

[9]R. Tycko, Phys. Rev. Lett. **58**, 2281 (1987).

[10]There is some subtlety involved. The basic principle of quantum mechanics asserts that if a state is an energy eigenstate with energy E its wave function depends on time according to e^{-iEt}. Here the time dependence of the states is not of the form e^{-iEt} and in fact is subject to experimental control. With a time-dependent Hamiltonian, energy is not, strictly speaking, a useful concept because the external agent causing the time dependence is doing work on the system. Rather, one should enlarge the Hamiltonian to include the external agent which makes the Hamiltonian time dependent, as for example in the treatment of molecular dynamics in the Born-Oppenheimer approximation. We should couple in an external electromagnetic field and compute its frequency shift. Alternatively, we can quantize the effective Lagrangian describing the dynamics of θ and φ and incorporating the phase shift (as outlined in Ref. 4).

[11]M. Forgacs and N. Manton, Commun. Math. Phys. **72**, 15 (1980). We thank Y. S. Wu for calling our attention to this reference. See also E. Witten, Phys. Rev. Lett. **38**, 121 (1977); Gu Chaohao, Phys. Rep. **80**, 251 (1981).

[12]The trace of a 2×2 simple unitary matrix determines the matrix up to a unitary transformation, of course. Thus three loops are needed here. In general, only two loops are needed.

[13]A. Pines (private communication).

[14]T. T. Wu and C. N. Yang, Nucl. Phys. B **107**, 365 (1976).

[15]Another way of seeing this point is to note that (for spin $\frac{1}{2}$) the instantaneous state η defined in the text is equal to $[e^{(-i\varphi/2)}\cos(\theta/2),\ e^{(i\varphi/2)}\sin(\theta/2)]$ and thus undefined at the poles. In contrast $\eta'=e^{(i\varphi/2)}\eta$ is undefined only at the south pole.

[16]A similar phenomenon has been discussed by L. Brown and W. Weisberger Nucl. Phys. B **157**, 285 (1979); with the gauge potentials $A=(-i)(\sigma_1 dx+\sigma_2 dy)/2$ and $A'=(-i)\sigma_3(dy/2)$ in two-dimensional Euclidean space.