Berry Phase for Systems with Angular Momenta in Electric and Magnetic Fields

K.J.B. Ghosh, D. De Munshi and B. Dutta-Roy

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Abstract

The Berry phase for a variety of systems comprising of two angular momenta is discussed. These include the electron and proton in the ground state of the hydrogen atom (taking into account the hyperfine interaction), the positronium atom ($^3S_1$ and $^1S_0$ states), the $\mu^+e^+$ and $\mu^+\mu^-$ bound states, the spin and orbital angular momenta of a single electron, $\mu^-$ capture by the deuteron in an external magnetic field, etc. Though the time scales involved, the underlying intrinsic Hamiltonians are quite different, as also the possible experimental probes, the geometric nature of the results for the Berry phase due to a time varying externally imposed magnetic field is found to be quite robust. Some indications are also put forward as to the possible interesting studies with time varying electric fields. The objective of this work is an attempt to broaden the scope of such studies in both the experimental and theoretical directions.
1 Introduction

The effect of Berry phase can be found in a variety of systems such as in optics, especially polarization of light (ref. [9],[10],[11]), molecular spectroscopy [12], atom-molecule scattering [13], nuclear quadrupole resonance [2], quantum Hall effect [14] and many other fields ranging from optics to condensed matter physics to atomic and molecular physics. Hence understanding of Berry phase enables one to comprehend a variety of phenomena observed in diverse fields of study.

Even though the concept of Berry phase [1] arose most naturally with the physical setting of a state of a quantum system with a time dependent Hamiltonian, where the adiabatic approximation can be applied, whereby the state clings to the instantaneous eigenstate of the changing Hamiltonian, nevertheless it emerges as an important intrinsic geometric property of the state in question, in the space of parameters that characterize the time dependence of the Hamiltonian. The Berry phase $\gamma_n(t)$ manifests itself as an extra phase factor in the eigenfunction of the instantaneous Hamiltonian (with eigenvalue $E_n(t)$) over and above the familiar dynamical phase $-\frac{\hbar}{\pi} \int_0^t E_n(t')dt'$. Thus even if the change in the Hamiltonian is cyclic so that $H(t=T) = H(t=0)$ a non-integrable phase factor $\gamma_n(T)$ for the eigenfunction remains as an anholonomy. Moreover $\gamma_n(T)$ can be expressed in terms of the solid angle (or its generalization) of the path (circuit) executed in parameter space (through time $t=0$ to $T$) subtended at the point in the parameter space where the degeneracies lifted by the time dependent part of the Hamiltonian are restored (known as the "diabolical point"). This is the geometric aspect of the Berry phase. In analogy with the phase that the wavefunction of a charged particle acquires upon execution of a closed path in a magnetic field, which is related to the flux enclosed by that circuit, one can also associate an underlying gauge field with the Berry phase (ref [3],[4]). Depending on whether the state (labeled here by $n$) of the system under consideration being 'transported', so to say, is non-degenerate or degenerate, the underlying gauge field is Abelian or Non-Abelian.

For concreteness (and also for relevance to the present study), we focus on a particle (or system of particles) with angular momenta and associated magnetic moments (with corresponding gyromagnetic ratios) in an external time dependent magnetic field $\vec{B}(t)$. Thus the Hamiltonian governing the time dependence of the system is itself time-dependent, as encoded in the three dimensional parameter space (in this case) describing the magnetic field. Furthermore, let us for instance allow the magnetic field to vary with time in such a manner as to keep its magnitude and polar angle fixed but
its azimuth ($\phi$) increasing uniformly with time with some angular frequency ($\omega$) such that $\phi = \omega t$ and

$$\vec{B} = B_0 (\sin \theta \cos \phi \hat{i} + \sin \theta \sin \phi \hat{j} + \cos \theta \hat{k})$$  \hspace{1cm} (1)$$

Thus the magnetic field vector, in the parameter space traces out in time a cone with a semi-vertical angle $\theta$. The Berry phase was found in the case of a spin half particle, to be determined by the solid angle $\Omega_c$ subtended at $\vec{B} = 0$ (the point in the parameter space where the Zeeman splitting vanishes) by the closed curve traced out in that space by the tip of $\vec{B}$ after one cycle of evolution viz. $T = \frac{2\pi}{\omega}$. For the particular case at hand (Eq. 1), this solid angle is given by $\Omega_c = 2\pi (1 - \cos \theta)$ and for the states of the particle of spin half, the Berry phase is given by $\gamma_m(C) = -m\Omega_c$ with $m = \pm \frac{1}{2}$ for the two states. Moreover, the generalization of the results to the case of the arbitrary angular momentum $j$ is readily accomplished and simply yields $\gamma_m(C) = -m\Omega_C$ with $m = -j.....+j$.

More recently there have been papers (ref \[5\],\[6\],\[7\]) devoted to the Berry phase under the conditions similar to what has been described above, for a system of two identical spin half particles keeping in mind relevance to the entangled states in context the of Quantum Information Theory. One of the points we wish to emphasize in the present study is the robustness of Berry’s result not only for the case of two identical spin one-half particles but for a more general scenario where the particles are non-identical and carry different gyro-magnetic ratios. Indeed the results seem to be more group theoretical than geometrical. The main difference in the generic structure of the two situations arises from the fact that in the case of identical particles, the interaction Hamiltonian with the magnetic field is symmetric under the exchange of the two spins and hence the magnetic field is incapable of causing , through its interaction, any admixture between spin singlet (antisymmetric under spin exchange) and spin triplet (symmetric under spin exchange) states. Thus the basic nature of the interaction Hamiltonian in the case of non-identical particles is quite different. The second aspect of our study pertains to the variety of such systems of two spin one-half particles, representing a vast range of energy and timescales, as also the diversity of the underlying experimental techniques and probes for investigation. Thus, for example, one may consider the positronium atom composed of the electron and the positron in the two lowest $^1S_0$ (para) and $^3S_1$ (ortho) states, each having their own distinctive decay modes into two and three gammas with lifetimes $10^{-10}$ and $10^{-7}$ seconds respectively. This system, in the present context, is the very antithesis of the case of two identical electrons, because
here the interaction with the magnetic field is antisymmetric under the exchange of spins because the gyromagnetic ratios of the electron and positron are equal in magnitude and opposite in sign. Another example at the other extreme of the time and energy scale are the lowest hyperfine interaction split triplet and singlet states of the hydrogen atom where the transition between the former and the latter states gives rise to the famous 21 cm line of the electromagnetic spectrum and has a lifetime of approximately ten million years! Another amusing set of examples involve the muon (which has a lifetime of 2.2 microseconds), such as the $\mu^+ e^- , \mu^- e^+$ and $\mu^+\mu^-$ bound states. Here an interesting experimentally exploitable feature is the fact that through its parity violating weak decay, the muon self-analyses its state of polarization, through the angular distribution of its decay electrons.

2 System with Two Angular Momenta in a Time Varying Magnetic Field

2.1 Systems with Two Spin One-Half Particles

The generic Hamiltonian under study is

$$H = G(\vec{S}_1 \cdot \vec{S}_2) - \mu_B \vec{B}(t) \cdot (g_1 \vec{S}_1 + g_2 \vec{S}_2)$$

where $G$ is the strength of the 'hyperfine' interaction between the two spins, $\mu_B = \frac{e}{2mc}$ is the Bohr magneton with $m = m_e$ for electron, $m = m_p$ for proton and $m = m_\mu$ for muon and $g_1$ and $g_2$ are the gyromagnetic ratios of the two particles involved. X.C. Tang et.al. (ref [7]) confining their attention to the system of two identical particles (the special case with $g_1 = g_2$), in the rotating magnetic field (Eq.1) found that here too Berry’s result for the phase was obtained if the quantum number (there for a single particle) is replaced by that of the respective entangled state. In the more general scenario that we are considering, it is convenient to introduce the total angular momentum $\vec{S} = \vec{S}_1 + \vec{S}_2$ and the difference angular momentum $\Delta \vec{S} = \vec{S}_1 - \vec{S}_2$ and to rewrite the Hamiltonian as

$$H = \frac{G}{2}(S^2 - S_1^2 - S_2^2) - \mu_B B_0 g_+ \left[ \frac{1}{2} \sin \theta (S_+ e^{-i\phi} + S_- e^{-i\phi}) + \cos \theta S_z \right]$$

$$- \mu_B B_0 g_- \left[ \Delta S_x \sin \theta \cos \phi + \Delta S_y \sin \theta \sin \phi + \Delta S_z \cos \theta \right]$$

where we have introduced $g_\pm = \frac{1}{2}(g_1 \pm g_2)$ and the ladder operators $S_\pm = S_x \pm iS_y$. Since we have two spin one-half particles a natural choice of the basis states are the singlet ($|0,0>$) and the triplet ($|1,1>, |1,0>, |1,-1>$).
states. If \( g_- = 0 \) (the case of identical particles) the matrix elements of the Hamiltonian connecting the singlet and the triplet states are zero. In general \( g_- \neq 0 \) (the case we are considering) and the structure of the Hamiltonian is much more interesting, since coupling between the singlet and the triplet states are permitted.

The following equations give the eigenvalues and eigenvectors of \( H \) respectively

\[
E_1 = \frac{\eta}{2} + \gamma_+
\]

\[
|n_1 > = \frac{1}{\sqrt{2}} \sin \theta e^{i\phi} |1, 0 > + \frac{1}{2} (1 - \cos \theta) e^{2i\phi} |1, -1 > + \frac{1}{2} (1 + \cos \theta) |1, 1 >
\]

\[
E_2 = \frac{\eta}{2} - \gamma_+
\]

\[
|n_2 > = \frac{1}{\sqrt{2}} \sin \theta e^{-i\phi} |1, 0 > - \frac{1}{2} (1 - \cos \theta) |1, -1 > + \frac{1}{2} (1 + \cos \theta) e^{-2i\phi} |1, 1 >
\]

\[
E_3 = -\frac{\eta}{8} + k
\]

\[
|n_3 > = \cos \chi |0, 0 > - \sin \chi \cos \theta |1, 0 > - \frac{1}{\sqrt{2}} \sin \chi \sin \theta e^{i\phi} |1, -1 > + \frac{1}{\sqrt{2}} \sin \chi \sin \theta e^{-i\phi} |1, 1 >
\]

\[
E_4 = -\frac{\eta}{8} - k
\]

\[
|n_4 > = \sin \chi |0, 0 > + \cos \chi \cos \theta |1, 0 > + \frac{1}{\sqrt{2}} \cos \chi \sin \theta e^{i\phi} |1, -1 > - \frac{1}{\sqrt{2}} \cos \chi \sin \theta e^{-i\phi} |1, 1 >
\]

where,

\[
\eta = G \hbar
\]

\[
\gamma_\pm = -\mu_B B_0 g_\pm
\]

\[
tan \chi = \frac{\gamma_-}{\frac{\eta}{8} + k}
\]

\[
k = \sqrt{\left(\frac{3\eta}{8}\right)^2 + (\gamma_-)^2}
\]
The geometric phase for the nth eigenstate is given as-

$$\gamma_n = i \oint <n(R)|\nabla_R n(R)> dR \tag{12}$$

The circuit integral is in the parameter space where the hamiltonian is varied adiabatically. In our system the variable parameter is $\phi$. Hence Eq. \ref{12} becomes-

$$\gamma_n = i \int_0^{2\pi} <n(\phi)|\frac{\partial}{\partial \phi} n(\phi)> d\phi \tag{13}$$

Applying the above formula to the eigenstates of $H$, we get,

$$\gamma_{n_1} = -2\pi(1 - \cos \theta) \tag{14}$$
$$\gamma_{n_2} = 2\pi(1 - \cos \theta) \tag{15}$$
$$\gamma_{n_3} = 0 \tag{16}$$
$$\gamma_{n_4} = 0 \tag{17}$$

2.2 Systems with One Spin 1 and One Spin $\frac{1}{2}$ Angular Momenta

The system of one spin 1 and one spin half particle is also of importance in several scenarios. It can describe spin orbit coupling of electrons in the first excited state of atoms of alkali metals (or singly charged alkali earth metal ions), as well as hyperfine interaction between electron in the ground state of a deuterium atom and its nucleus.

We take the Hamiltonian same as Eq.\ref{3} (in the case where the spin one corresponds to the orbital angular momenta the gyromagnetic ratio is 1). For a system of two angular momenta, one and one-half, the natural choice of the basis states are $|\frac{3}{2}, \frac{3}{2}>, |\frac{3}{2}, \frac{1}{2}>, |\frac{3}{2}, -\frac{1}{2}>, \text{ and } |\frac{3}{2}, -\frac{3}{2}>$, which we call the quartet states and $|\frac{1}{2}, \frac{1}{2}>, |\frac{1}{2}, -\frac{1}{2}>$, which we call the doublet states.

The following table gives the Berry phase for the eigenstates of the Hamiltonian (Eq.\ref{3})
where, 

\[ \eta = Jh \]
\[ \gamma_\pm = -\mu_B B_0 h \gamma_\pm \]

\[ k^2 = \frac{(\gamma_+ + 3\gamma_-)(\gamma_+ + \gamma_-)}{(\gamma_+ + \frac{5\gamma_-}{3})(\gamma_+ + \frac{2\gamma_-}{3})} \]

3 Systems with Electric Quadrupole Moment in a Time Varying Electric Field

To discuss the electrical analogue of the problem considered so far, it is suitable to express the electric quadrupole moment operator (a second rank symmetric tensor) as built up from the angular momentum vector, viz.,

\[ Q_{ik} = \frac{1}{2}(J_i J_k + J_k J_i) - \frac{1}{3} \delta_{ik} \vec{J} \cdot \vec{J} \]  \hspace{1cm} (18)
As such the $Q_{z'z'}$ component (with $z'$ the time dependent direction along which the $z'$ component of the electric field has a gradient $q_0$) of this tensor is given by

$$Q_{z'z'} = J^2_{z'} - \frac{1}{3} J^2$$

which with

$$J_{z'} = J_x \sin \theta \cos \phi + J_y \sin \theta \sin \phi + J_z \cos \theta$$

will, with $\theta$ fixed and $\phi = \omega t$, provide us with the electric correspondence of the magnetic field vector executing gyration along a cone. Thus we have

$$Q_{z'z'} = J^2_x (\sin^2 \theta \cos^2 \phi - \frac{1}{3}) + J^2_y (\sin^2 \theta \sin^2 \phi - \frac{1}{3})$$

$$+ J^2_z (\cos^2 \theta - \frac{1}{3}) + (J_x J_y + J_y J_x) \sin^2 \theta \cos \phi \sin \phi$$

$$+ (J_y J_z + J_z J_y) \sin \theta \cos \theta \sin \phi + (J_z J_x + J_x J_z) \sin \theta \cos \theta \cos \phi$$

The Hamiltonian of the interaction of the quadrupole moment of the system with the ‘rotating’ electric field gradient is (taking into account factors arising from the Taylor expansion of the electric potential and the conventional definition of the electric quadrupole moment $Q$) given by

$$H_{int} = \left( \frac{e^2 q_0 Q}{12} \right) (J^2_{z'} - \frac{1}{3} J^2)$$

Let us for concreteness consider the simplest example of a particle with spin $j = 1$ (for instance the deuteron). The eigenstates of $J_{z'}$ belonging to eigenvalues $+1$, $-1$ and $0$, written in the basis in which $J_z$ is diagonal are

$$|\chi_{+1}\rangle = \frac{1}{2}(1+\cos \theta)e^{-i\phi}|1,1\rangle + \frac{1}{\sqrt{2}} \sin \theta |1,0\rangle + \frac{1}{2}(1-\cos \theta)e^{+i\phi}|1,-1\rangle$$

$$|\chi_{-1}\rangle = \frac{1}{2}(1-\cos \theta)e^{-i\phi}|1,1\rangle - \frac{1}{\sqrt{2}} \sin \theta |1,0\rangle + \frac{1}{2}(1+\cos \theta)e^{+i\phi}|1,-1\rangle$$

$$|\chi_0\rangle = \frac{1}{\sqrt{2}} \sin \theta e^{-i\phi}|1,1\rangle + \cos \theta |1,0\rangle + \frac{1}{\sqrt{2}} \sin \theta e^{+i\phi}|1,-1\rangle$$
These are of course automatically also eigenstate of $H$ but while, \( |\chi_0 > \) is an eigenvector of $H$ belonging to the eigenvalue \(-\left( \frac{e^2q_0Q}{12} \right)^{\frac{1}{3}}\), the vectors \(|\chi_{+1} >\) and \(|\chi_{-1} >\) are both eigenvectors of $H$ belonging to the eigenvalue \( \left( \frac{e^2q_0Q}{12} \right)^{\frac{1}{3}}\), and hence we have here a two fold degeneracy. While for the state \(|\chi_0 >\), the Berry phase may be obtained as earlier, since the instantaneous eigenstates \(|\chi_{+1} >\) and \(|\chi_{-1} >\) are degenerate, it is unclear whether true adiabatic change is possible for these two states. However, since the change being made is through rotation about the Z-axis, the states, which are eigenstates of $J_z$, are the proper linear combination in the manifold of degenerate states, for which the phase matrix is diagonalized, and consequently the notion of Berry’s phase remains meaningful, as discussed by Wilczek and Zee, and Simon (ref. [3],[8]) .

However, $J_z$ can be expressed as a linear combination of $J_x'$, $J_y'$ and $J_z'$, and hence of $J_{+}'$, $J_{-}'$ and $J_z'$. But since these operators can only cause a change in the projection quantum number $\Delta m' = 0, \pm 1$, it is only in the Kramer’s degenerate subspace $\pm \frac{1}{2}$ that the non-abelian nature of the underlying gauge group manifests itself in a non-trivial manner. Indeed, in the degenerate subspaces, $\pm m$ other than the case $m = \frac{1}{2}$, the eigenstates of $J_z'$ are automatically also the eigenstates of $J_z$.

The Berry phases for a spin 1 particle in an electric field with a rotating field gradient is given as follows- 

| Eigenstates | Energy Eigenvalues | Eigenphase |
|------------|--------------------|------------|
| $|\chi_{+} >$ | $(\frac{e^2q_0Q}{12})^{\frac{1}{3}}$ | $2\pi\cos\theta$ |
| $|\chi_{-} >$ | $(\frac{e^2q_0Q}{12})^{\frac{1}{3}}$ | $-2\pi\cos\theta$ |
| $|\chi_{0} >$ | $-(\frac{e^2q_0Q}{12})^{\frac{1}{3}}$ | $\pi(1 - \cos\theta)$ |

4 Conclusion

In this exercise we have tried to investigate the effect of a time dependent Hamiltonian for two particle systems, concentrating on time dependent magnetic field effects on the Berry phase of two coupled spin half particles and one spin one-half and spin one particle coupled together. Such a study gave
us an opportunity to go back to the original work of Berry and discover that the statement made by Berry regarding the phase of the wavefunction of a spin one-half particle in a rotating magnetic field has a general validity even for systems with two particles. Hence we might be able to hypothesize that the formula $2\pi m(1 - \cos \theta)$ will be correct for systems with greater number of particles with different values of spin, where in those cases, $m$ will refer to the value of $S_z$ component along the direction of the magnetic field, $S_z$ being the $z$ component of the total angular momentum of the particles.

In our quest to broaden the range of physical systems where the Berry phase may manifest itself, we have considered electric field analogues of the above situation. Here, because of the Kramer’s degeneracy, among states of angular momentum projection ($\pm m$), stemming from time-reversal invariance, Wilczek and Zee pointed out the relevance of a non-abelian gauge field underlying these phases. This has led to an experimental verification in the case of the levels of a nucleus of spin $\frac{3}{2}$ in the electric field gradients due to the crystalline field of a rotating solid sample (ref.[2]). We discussed the generalized scenario starting from the simplest $j = 1$ situation. For both time varying magnetic and electric fields, we point out the gauge variety of systems involving a vast range of timescales and the use of a diversity of techniques and possibly several amusing manifestations of the Berry phase posing challenges to experimental technology. Lastly it is important to underline the fact that in the kind of problems being brought forth in the point of view we advocate, those involved in the very basis of quantum mechanics, physics of atoms and molecules, solids, nuclei and elementary particles can share a common platform of investigation.

5 References

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