PRAMANA
—journal of
physics

© Printed in India

Vol. 49, No. 1,
July 1997
pp. 33–40

The quantum geometric phase as a transformation invariant

N MUKUNDA*
Centre for Theoretical Studies and Department of Physics, Indian Institute of Science, Bangalore 560 012, India
* Honorary Professor, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560 064, India

Abstract. The kinematic approach to the theory of the geometric phase is outlined. This phase is shown to be the simplest invariant under natural groups of transformations on curves in Hilbert space. The connection to the Bargmann invariant is brought out, and the case of group representations described.

Keywords. Geometric phase; Bargmann invariant.

PACS No. 03.65

1. Introduction

Ever since Berry's important work of 1984 [1], the geometric phase in quantum mechanics has been extensively studied by many authors. It was soon realised that there were notable precursors to this work, such as Rytov, Vladimirskii and Pancharatnam [2]. Considerable activity followed in various groups in India too, notably the Raman Research Institute, the Bose Institute, Hyderabad University, Delhi University, the Institute of Mathematical Sciences to name a few.

IIn the account to follow, a brief review of Berry's work and its extensions will be given [3]. We then turn to a description of a new approach which seems to succeed in reducing the geometric phase to its bare essentials, and which is currently being applied in various situations [4]. Its main characteristic is that one deals basically only with quantum kinematics. We define certain simple geometrical objects, or configurations of vectors, in the Hilbert space of quantum mechanics, and two natural groups of transformations acting on them. We then seek the simplest expressions invariant under these transformations. This is seen to lead immediately to a kinematic view of the geometric phase. It helps us pose useful questions and connect the phase to other more familiar expressions in quantum mechanics.

2. Quantum kinematics: States, phases and rays

As is well-known, in the quantum mechanical description of any system the dynamical variables are linear operators on a suitably constructed Hilbert space $\mathcal{H}$, while the various (pure) states of the system correspond to vectors $\psi, \psi', \ldots$ in $\mathcal{H}$. The superposition principle of quantum mechanics permits us to form linear combinations $c_1\psi_1 + c_2\psi_2 \ldots$ of given vectors $\psi_1, \psi_2 \ldots$ using complex coefficients $c_1, c_2 \ldots$, and thus to produce new pure states from old ones in a completely nonclassical way. (This is of course apart from superselection rules.) The relation between vectors and physical states is quite subtle. Namely, a change in the overall phase of a vector in $\mathcal{H}$, $\psi \rightarrow e^{i\alpha}\psi$, causes no change in the physical state at all. Thus the relation between vectors in $\mathcal{H}$ and distinct physical states is many-to-one. One is thus motivated to introduce the concept of rays [5] – equivalence classes of vectors differing from one another by phases alone–so that between rays and physical states the relation is one-to-one. A given vector $\psi \in \mathcal{H}$ determines a corresponding ray consisting of all the vectors $e^{i\alpha}\psi$, $0 \leq \alpha < 2\pi$; this ray can be conveniently represented by the pure state density matrix or projection operator onto ψ, namely $\rho = \psi\,\psi^\dagger$, and one has these relationships:

$$\begin{aligned}
&\text{Vectors } \psi \text{ in } \mathcal{H} \xrightarrow{\text{many-to-one}} \text{physical states;}\\
&\text{Vectors } \psi \text{ in } \mathcal{H} \xrightarrow{\text{quotient w.r.t } U(1)} \text{rays } \rho = \psi\,\psi^\dagger;\\
&\text{rays } \rho = \psi\,\psi^\dagger \xrightarrow{\text{one-to-one}} \text{physical states.}
\end{aligned} \tag{1}$$

The geometry of ray space is somewhat complicated, and not as easy to visualize as that of $\mathcal{H}$. Moreover the superposition principle is not manifest, though it is certainly present. Nevertheless, its use is crucial not only in the above context but also for the geometric phase.

In contrast to overall phases being unobservable, relative phases in a linear combination, such as in $\psi_1 + e^{i\alpha}\psi_2$, are physically observable – all quantum mechanical interference phenomena ultimately have their origins in such relative phases.

We shall hereafter deal with unit vectors in $\mathcal{H}$, namely with points on the unit sphere in $\mathcal{H}$, and will not mention this repeatedly.

3. Quantum dynamics, adiabatic theorem and the geometric phase

Quantum dynamics is governed by the time-dependent Schrodinger equation: for each t we have a vector $\psi(t) \in \mathcal{H}$ evolving according to

$$i\hbar\frac{d}{dt}\psi(t) = H(t)\psi(t). \tag{2}$$

Here $H(t)$ is the Hamiltonian operator of the system, and the possible explicit time dependence allows for external or environmental influences on the system. For a completely isolated system there would be no such dependence.

Berry's original discovery of the geometric phase was in the following context. Imagine a situation where $H(t)$ changes very slowly – adiabatically – with passage of time, and suppose for each time we have a nondegenerate normalized eigenvector $u(t)$

with corresponding eigenvalue $E(t)$:

$$H(t)\, u(t) = E(t) u(t). \tag{3}$$

Thus we have an instantaneous energy eigenstate with time-dependent energy. Then the Born–Fock adiabatic theorem of quantum mechanics [6] states that an approximate solution of the Schrodinger equation (2) is given by

$$\psi(t) \simeq \exp\left[\frac{-i}{\hbar}\int_0^t E(t')\mathrm{d}t'\right] u(t), \tag{4}$$

where the (hitherto) free phase factor in $u(t)$ is restricted by the convention

$$(u(t),\, \dot{u}(t)) = 0. \tag{5}$$

Now suppose we have a cyclic environment: $H(T) = H(0)$ for some time T. The question is whether, when the environment returns to its original condition, the state vector also does so. While it was long known that the physical state returns to its original form, the precise behaviour of the state vector had not been properly appreciated until Berry's work. What Berry found was that there was a new piece in the phase factor relating $\psi(T)$ to $\psi(0)$, which was geometrical in origin:

$$\begin{aligned} \psi(T) &\simeq \exp\left(\frac{-i}{\hbar}\varphi_{\text{tot}}\right)\psi(0), \\ \varphi_{\text{tot}} &= \varphi_{\text{dyn}} + \varphi_{\text{geom}}, \\ \varphi_{\text{dyn}} &= \int_0^T \mathrm{d}t\, E(t). \end{aligned} \tag{6}$$

The total phase φ_{tot} is made up of a dynamical part, already evident in eq. (4) expressing the adiabatic theorem, and a geometric piece φ_{geom} which cannot be transformed away. Indeed, one can see that a nontrivial geometric phase implies $u(T) \neq u(0)$ if eq. (5) is obeyed.

Thus the geometric phase was originally found in the context of adiabatic, cyclic unitary evolution governed by the Schrödinger equation. Later developments showed that each of the first three conditions could be relaxed [7] – thus the geometric phase could be usefully defined even for nonadiabatic, noncyclic, nonunitary evolution governed by the Schrödinger equation. The developments to be now described show that one can even dispense with the Schrödinger equation!

4. The kinematic approach

On the unit sphere in $\mathcal{H}$ we define the following geometric objects: Open smooth parametrized curves $\mathcal{C}$, which may be pictured as strings lying on the sphere. Such a curve $\mathcal{C}$ may be represented as a collection of vectors in this way:

$$\mathcal{C} = \{\psi(s),\ \ s_1 \leq s \leq s_2\}. \tag{7}$$

The end points are $\psi(s_1)$ and $\psi(s_2)$; and while $\psi(s)$ must vary continuously with no breaks, a finite number of points where it is not differentiable can be tolerated.

Two groups of transformations can be defined to act on these curves, mapping each $\mathcal{C}$ to another $\mathcal{C}'$:

(i) Local phase changes:

$$\begin{aligned} \mathcal{C} \rightarrow \mathcal{C}' : \psi(s) \rightarrow \psi'(s) &= e^{i\alpha(s)}\psi(s), \\ \alpha(s) &= \text{smooth function of } s. \end{aligned} \tag{8}$$

(ii) Monotonic reparametrizations:

$$\begin{aligned} s' &= f(s), \quad \dot{f}(s) > 0, \\ \psi'(s') &= \psi(s). \end{aligned} \tag{9}$$

If we denote the ray space image of $\mathcal{C}$ by C, it is clear that the local phase changes do not alter this image at all. The reparametrization transformation traverses the same set of points but at an altered rate; so the set of points comprising $\mathcal{C}$ receives a new description. The same is then true of C as well.

We now ask for the simplest functional of $\mathcal{C}$ with the property that it is invariant under both these transformations. With a little bit of work, one easily finds that the following expression is doubly invariant [8]:

$$\varphi_g = \arg(\psi(s_1), \psi(s_2)) - \int_{s_1}^{s_2} \mathrm{d}s \,\mathrm{Im}(\psi(s),\ \dot{\psi}(s)). \tag{10}$$

This is the geometric phase associated with C! We see that it is the difference of two terms, each individually dependent on $\mathcal{C}$. However local phase invariance means that φ_g is really a functional of the ray space image C of $\mathcal{C}$; and the reparametrization invariance indicates its geometric nature. All this can be expressed as follows:

$$\begin{aligned} \varphi_g[C] &= \varphi_{\mathrm{p}}[\mathcal{C}] - \varphi_{\mathrm{dyn}}[\mathcal{C}], \\ \varphi_{\mathrm{p}}[\mathcal{C}] &= \arg(\psi(s_1), \psi(s_2)) \\ \varphi_{\mathrm{dyn}}[\mathcal{C}] &= \int_{s_1}^{s_2} \mathrm{d}s\ \mathrm{Im}(\psi(s),\ \dot{\psi}(s)). \end{aligned} \tag{11}$$

The term $\varphi_{\mathrm{p}}[\mathcal{C}]$ – the subscript standing for Pancharatnam – is just the total phase seen in eq. (6). It depends only on the end points of $\mathcal{C}$ and is in that sense a nonlocal quantity. The term $\varphi_{\mathrm{dyn}}[\mathcal{C}]$ is the 'dynamical' piece – it is an integral along $\mathcal{C}$ of a locally defined integrand.

Given any smooth curve C in ray space, we may choose *any* lift $\mathcal{C}$ in $\mathcal{H}$ projecting onto C. Then the calculation of the quantities $\varphi_{\mathrm{p}}[\mathcal{C}]$ and $\varphi_{\mathrm{dyn}}[\mathcal{C}]$ dependent on $\mathcal{C}$ is immediate. Their difference however is independent of the particular lift $\mathcal{C}$ and depends on C alone. In all this we see how easy it is to deal with open curves in Hilbert or ray space-noncyclic evolution. Whereas $\varphi_{\mathrm{dyn}}[\mathcal{C}]$ is the integral along $\mathcal{C}$ of a suitably defined one-form on $\mathcal{H}, \varphi_g[C]$ cannot be displayed in any similar fashion at ray space level.

Particular kinds of lifts $C \rightarrow \mathcal{C}$ can lead to corresponding simplifications:

(i) Horizontal lifts: Here $(\psi(s),\ \dot{\psi}(s)) = 0$ throughout, so one has

$$\varphi_{\mathrm{dyn}}[\mathcal{C}] = 0, \quad \varphi_g[C] = \varphi_{\mathrm{p}}[\mathcal{C}]. \tag{12}$$

(ii) Pancharatnam lifts: Now the end points are chosen to be 'in phase' in the Pancharatnam sense, so that $(\psi(s_1),\ \psi(s_2))$ is real positive, and then

$$\begin{aligned}\varphi_{\mathrm{p}}[\mathcal{C}] &= 0,\\ \varphi_g[C] &= -\varphi_{\mathrm{dyn}}[\mathcal{C}].\end{aligned} \tag{13}$$

One can ask for an expression for $\varphi_g[C]$ directly in terms of density matrices, not involving state vectors at all. One such expression which shows clearly the 'nonlocal' dependence of $\varphi_g[C]$ on C is

$$\varphi_g[C] = \arg\ \mathrm{Tr}\left\{\rho(s_1)\,P\left(\exp\int_{s_1}^{s_2}\mathrm{d}s\,\frac{\mathrm{d}\rho(s)}{\mathrm{d}s}\right)\right\}. \tag{14}$$

Reparametrization invariance and the geometric nature are evident.

All the earlier treatments and special cases can be easily recovered from this formalism. In the case where one is dealing with some solution of the Schrödinger equation for some given Hamiltonian, one can clearly pose and answer interesting questions: how does the geometric phase behave under static and dynamic symmetries of the Hamiltonian and under antiunitary time reversal? It turns out to be invariant under both static symmetries and time reversal, but in general not under dynamic symmetries [8].

5. Connection to the Bargmann invariants

Given any continuous curve $\mathcal{C}$ of unit vectors in $\mathcal{H}$, with image C in ray space, it is possible to define the 'length' of C as a functional of C. By extremising this functional one arrives at the concept of geodesics in ray space. For convenience, *any* lift of a ray space geodesic will be regarded as a geodesic in Hilbert space as well. Then after suitable choices of phases and parametrization, it turns out that the most general geodesic in $\mathcal{H}$ is describable as follows [8]

$$\begin{aligned}&\psi(s) = \phi_1\cos s + \phi_2\sin s,\\ &(\phi_1,\phi_1) = (\phi_2,\phi_2) = 1, \quad (\phi_1,\phi_2) = 0.\end{aligned} \tag{15}$$

So it is basically a *real plane curve*, an arc of a circle in two dimensions. We see that phases and the complex nature of $\mathcal{H}$ are all absent here. As a consequence we obtain the key result [8]

$$\varphi_g[\text{geodesic } C \text{ in ray space}] = 0. \tag{16}$$

We now explain how this may be exploited.

If $\psi_1,\ \psi_2,\ldots,\psi_n$ are any n unit vectors in $\mathcal{H}$, given in this sequence, they define the Bargmann invariant [9]

$$\begin{aligned}\Delta_n(\psi_1,\psi_2,\ldots,\psi_n) &= (\psi_1,\psi_2)(\psi_2,\psi_3)\cdots(\psi_{n-1},\psi_n)(\psi_n,\psi_1)\\ &= \mathrm{Tr}\,(\rho_1\rho_2\cdots\rho_n),\\ \rho_1 = \psi_1\psi_1^\dagger,&\quad \rho_2 = \psi_2\psi_2^\dagger,\ldots.\end{aligned} \tag{17}$$

The context in which Bargmann introduced such expressions (for the case $n = 3$) was a discussion of the Wigner unitary–antiunitary theorem [10]: any symmetry in quantum mechanics, i.e., any probability preserving map of (pure state) rays on to rays, can be lifted to either a linear unitary or an antilinear antiunitary map at the Hilbert space level. The behaviour of Δ_3 distinguishes between these two alternatives, since it is invariant in the unitary case and goes to its complex conjugate in the antiunitary case.

The link between geometric phases and Bargmann invariants arises from the result (16) for geodesics. Given the points or vertices $\psi_1, \psi_2, \ldots, \psi_n$ needed to set up Δ_n, join ψ_1 to ψ_2 by a geodesic arc, ψ_2 to ψ_3 by another geodesic arc, and so on all the way till the geodesic arc from ψ_n back to ψ_1. This gives us an n-sided polygon in ray space as well, with $\rho_1, \rho_2, \ldots, \rho_n$ for vertices. We then find

$$\begin{aligned}\varphi_g \quad & [n\text{-sided polygon with vertices } \rho_1, \rho_2, \ldots, \rho_n] \\ &= -\arg \Delta_n(\psi_1, \psi_2, \ldots, \psi_n).\end{aligned} \tag{18}$$

This is a nice connection between something old and something new, and it also gives some feeling for the nature of the geometric phase. It can and has been used in several ways: for instance the original definitions (10, 11) for $\varphi_g[C]$ can be recovered by a limiting process via a polygonal approximation to C, showing how the pieces $\varphi_p[C]$ and $\varphi_{dyn}[C]$ arise respectively from the last and the previous factors in $\Delta_n(\psi_1, \psi_2, \ldots, \psi_n)$; it has been shown that the very well-known Guoy phase in classical beam optics is an instance of the geometric phase, as seen via the Bargmann invariant [11].

6. The case of Lie group representations

The next major application of this formalism is to a study of geometric phases arising out of unitary Lie group representations [12]. Many special features are present on account of the algebraic and differential geometric properties that now become available.

The framework we use is the following. We have a (compact or noncompact) Lie group G, with a faithful unitary representation $\mathcal{U}(\cdot)$ of it acting on a Hilbert space $\mathcal{H}$. The representation need not be irreducible. Denote its hermitian generators by $\{T_r\}$. We have a given fiducial vector $\psi_0 \in \mathcal{H}$. We are interested in calculating geometric phases for smooth curves C which start out at ψ_0 and are produced by continuous group action on ψ_0. It turns out that the dynamical part of the geometric phase can be studied in great detail and brought to a maximally simplified form. We indicate the structures and results briefly.

Given ψ_0 and the unitary representation $\mathcal{U}(g)$ of G on $\mathcal{H}$, two subgroups of G are naturally defined

$$\begin{aligned} H_0 &= \{g \in G | \mathcal{U}(g)\, \psi_0 = \psi_0\} \\ &= \text{stability group of } \psi_0; \\ H &= \{g \in G | \mathcal{U}(g)\psi_0 = (\text{phase factor})\psi_0\} \\ &= \text{stability group of } \psi_0 \text{ up to phases.} \end{aligned} \tag{19}$$

Clearly H_0 is an invariant subgroup of H. For definiteness we make the assumption that H_0 is compact – this is so in all physically interesting cases.

Now the curves $\mathcal{C}$ that we are interested in can be viewed or described in two ways: either as lying in the orbit $\mathcal{O}(\psi_0)$ of ψ_0 in $\mathcal{H}$, which consists of the collection of vectors $\mathcal{U}(g)\,\psi_0$ for all $g \in G$; or as lying in the coset space $M_0 = G/H_0$. This is because by a well-known argument these two objects are the same – there is a one-to-one correspondence between vectors $\psi \in \mathcal{O}(\psi_0)$ and cosets in G/H_0. Hence

$$\begin{aligned} \mathcal{C} &= \{\mathcal{U}(g(s))\psi_0 | g(s) \text{a smooth curve in } G\} \\ &= \text{curve in } G - \text{orbit } \mathcal{O}(\psi_0) \text{ of } \psi_0 \\ &= \text{curve in coset space } M_0 = G/H_0. \end{aligned} \tag{20}$$

To calculate the dynamical phase $\varphi_{\rm dyn}[\mathcal{C}]$, we need to appreciate that there are three (and only three) possible relations between H_0 and H, described as follows:

$$\begin{aligned} &\text{A)} \qquad H = H_0, \quad H/H_0 = \text{trivial}; \\ &\text{B)} \qquad H/H_0 = \text{discrete, nontrivial}; \\ &\text{C)} \qquad H/H_0 = U(1). \end{aligned} \tag{21}$$

In case (A) we are unable to change the phase of ψ_0 by group action, so $\mathcal{O}(\psi_0)$ consists of exactly one vector each from a certain collection of rays. In case (B) we can change the phase of ψ_0 by group action but only by certain discrete amounts, so $\mathcal{O}(\psi_0)$ consists of a discrete set of vectors drawn from each of a certain collection of rays. In case (C) we can change the phase of ψ_0 by any amount by suitable group action, so $\mathcal{O}(\psi_0)$ consists of a certain collection of entire rays. At the Lie algebra level, in cases (A) and (B), the subgroups H_0 and H have the same Lie algebra; while in case (C), H has an extra $U(1)$ generator invariant under H_0.

Now we turn to $\varphi_{\rm dyn}[\mathcal{C}]$. By using the Wigner–Eckart theorem of quantum mechanics, and following also the spirit of that theorem, we find we can simplify $\varphi_{\rm dyn}[\mathcal{C}]$ a great deal, and effect a neat separation of its algebraic and its geometric parts – namely, dependences on ψ_0, $\mathcal{U}(\cdot)$ on the one hand and dependence on $\mathcal{C}$ on the other. For this some standard differential geometric properties of G and M_0 are needed [13]. The Lie group G carries two sets of vector fields and their dual one forms, one set being left invariant and the other right invariant. These forms are the Maurer–Cartan one-forms and the Lie algebra structure can be expressed using either set. When we descend from G to the coset space $M_0 = G/H_0$, only some of the Maurer–Cartan forms survive and yield globally defined one-forms on M_0. These are the one-forms going with those generators of G which are scalar with respect to H_0. Using all this machinery and the standard Wigner–Eckart theorem we find

$$\varphi_{\rm dyn}[\mathcal{C}] = (\psi_0, T_\rho \psi_0) \int_{\mathcal{C}\subset M_0} \widehat{\theta}^\rho\,. \tag{22}$$

There is a sum here on the repeated index ρ : $\{T_\rho\}$ is a complete independent set of H-scalar generators among $\{T_r\}$, and $\widehat{\theta}^\rho$ are the pull-backs to M_0 of the Maurer–Cartan forms on G that are associated with the T_ρ. Among the $\{T_\rho\}$ we may omit any generators of H_0 since they annihilate ψ_0; and the $\widehat{\theta}^\rho$ are globally well-defined on M_0.

We see that $\varphi_{\rm dyn}[\mathcal{C}]$ is generally a sum of terms in each of which there is a neat separation of the algebraic representation dependent part from the geometric dependence on C. This simplified expression allows a systematic study and comparison of cases where $\mathcal{U}(g)$ may change but H_0 and C do not; when two groups G and G' are locally isomorphic but globally different, and the relevant coset spaces M_0, M_0' coincide, and so on.

Several applications of this formalism have been made: the Guoy phase was already mentioned, and this involves the metaplectic group $Mp(2)$; the case of $SU(3)$ representations including three-level quantum systems [14]; squeezing transformations etc. Indeed in practically every experimental realisation of geometric phases, it does happen that some Lie group is intimately involved!

7. Concluding remarks

This account conveys the value of viewing the geometric phase as a purely kinematic construct, and gives a new perspective on it. It has led to interesting questions and applications which are conceptually clear when expressed in the present framework. Lastly, as Feynman expressed himself in a well known paper: 'there is a pleasure in recognizing old things from a new point of view'.

References

[1] M V Berry, *Proc. R. Soc. (London)* **A392**, 45 (1984)
[2] S M Rytov, *Dokl. Akad. Nauk. (USSR)* **28**, 263 (1938)
V V Vladimirskii, *Dokl. Akad. Nauk (USSR)* **31**, 31 (1941)
S Pancharatnam, *Proc. Indian Acad. Sci.* **A44**, 247 (1956)
[3] See, for instance, A Shapere and F Wilczek, *Geometric phases in physics* (World Scientific Publishing Co. Pte. Ltd., Singapore, 1989)
[4] N Mukunda and R Simon, *Ann. Phys. (N.Y.)* **228**, 205, 269 (1993)
[5] H Weyl, *The theory of groups and quantum mechanics* (Dover Publications Inc., 1931) p. 4, 20
[6] See any standard text on quantum mechanics such as, for instance, L I Schiff, *Quantum Mechanics* (McGraw-Hill Book Company Inc., New York, 2nd edition, 1955) p. 213
[7] Y Aharonov and J Anandan, *Phys. Rev. Lett.* **58**, 1593 (1987)
J Samuel and R Bhandari, *Phys. Rev. Lett.* **60**, 2339 (1988)
[8] See the first of refs. [4] above
[9] V Bargmann, *J. Math. Phys.* **5**, 862 (1964)
[10] E P Wigner, *Group theory and its application to the quantum mechanics of atomic spectra* (Academic Press, New York, 1959) appendix to Ch. 20
[11] R Simon and N Mukunda, *Phys. Rev. Lett.* **70**, 880 (1993)
[12] See the second of refs. [4] above
[13] See, for instance, S Helgason, *Differential geometry and symmetric spaces* (Academic Press, New York, 1962)
B Schutz, *Geometrical methods of mathematical physics* (Cambridge University Press, London, 1980)
C J Isham, *Modern differential geometry for physicists* (World Scientific Publishing Co. Pte. Ltd., Singapore, 1989)
[14] G Khanna, S Mukhopadhyay, R Simon and N Mukunda, *Ann. Phys. (N.Y.)* **253**, 55 (1997)