Berry Phase: an Introduction

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Acknowledgments

This set of lecture notes accompanies prof. Mukundan Seminar course on Geometric Phase, taught from 10^{th} to 15^{th} March 2014.

The entire course is hosted on YouTube at the following address:

`https://www.youtube.com/playlist?list=PLhkiT_RYTEU15TB17zx32tbHGZ0mB6aSP`

These lecture notes are not endorsed by prof. Mukundan.

While I have tried to correct typos and errors made during the lectures (some helpfully pointed out by YouTube commenters), I have also taken the liberty to add and/or modify some of the material at various points in the notes. Any errors that may result from this are, of course, mine.

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Contents

1 Overview

The work is given by a total amount of 6 sections; this first introductory section is an overview of the subject. The second section is a discussion about the Berry original work: first as a sempilified form and then as it was originally presented by prof. Berry. The third section will be the generalization given by Aharonov and A. and a year later by Samuel and A. In that third section we eill introduce also a brief mathematical interlude and some geometrical consideration about curvature. The fourth section is devoted essentially to the so called Kinematic Approach and we will bring the concept of Bargman invariance and its connection to curvature and the interesting appliation to the entire formalisma. Fifth section will be a second mathematical interlude on simplectic and riemannian manifolds. Sixth section will be about the null phase idea.

2 Berry discovery of 1983-84

Berry discovery of 1983-84[1] was a new discovery on the context about adiabatic of quantum mechanics and this work initiated a lot of work worldwide. In Berry's derivation several independent assumptions were made: initially this phase was called the Berry Phase for everyone but over time this name changed to geometric phase and as we'll see this concept is relevant also in classical wave-optical situations. It's quite remarkable that there are some chances that this concept can be used in condensed matter context. On the other hand we hope that the way we're presenting this work can naturally point out the applications.

As we said many work have been done to relax the assumptions that Berry done in order to defend Berry's work under more general conditions. The first important step was taken by Aharonov and Anandan (1987). The second important by S and A was taken in 1988 and a third successful step was taken in 1993 and these are the successful and successive steps we'll describe. Apart from these improvements, people were also looking for earlier litteratures from different ideas much earlier then Berry. There are several of them but the most important we will touch upon is the on of PancharatnamPancharatnam (1956) in 1957, that is, 27 earlier than Berry work. The fact that the work of Pancharatnam was in the direction of the geometric phase was pointed out by ... and ... in 1986. The other important early work relevant in this subject was the one of Bargman and Valentine in 1964 mostly 20 years before Berry working on discuss inf Wigner theorem of 1931, a theorem that Wigner had proved on how symmetric operators can be represented in quantum mechanics. So the th itself is very early (1931); many people had tried to give alternative proof of Wigner Theorem and one very important is given by Bargman in 1964, particularly elegant. The fact that Bargman work was important in the discovery of the Berry phase was pointed out and exploited by Syman and auth. in 1993

These lectures will describe all these thing and more mathematical relevant structures in a more chronological structures, but will not be strictly chronological rigorous. You'll find that many features of QM which we we might be familiar with they will be re examined, re-defined from the geometrical phase pov. When we will come to the kinematic approach we will define some applications. This should give an overview and an idea of the scope of these lectures.

2.1 Simplified Form

We are now going to present the original Berry's work in a slightly simplified work.

[1] We say 1983-1984 since the original work was apparently submitted in 1983 but was at first instance rejected. However a preprint of his work must have been around since in 1983 another work on the Berry Phase appeared on Physical Review Letter. That's why sometimes the date can be misleading.

Having a quantum mechanical system in mind and a general setting, we will mainly deal with pure states $\mathscr{H}$ with a time dependent Hamiltonian $\mathcal{H}(t)$ governing the system and we have a state vector describing the system $\psi(t)$. The wavefunction must satisfy the (time dependent) Schrödinger equation

$$i\hbar\frac{d}{dt}\psi(t) = \mathcal{H}(t)\psi(t) \tag{2.1}$$ eq:2.1

If the Hamiltonian had be time independent, a formal solution of the Schrödinger equation is easy to find because what we have to do is to formally take the Hamiltonian and find out all its eigenfunctions and eigenvalues

$$\mathcal{H}\psi_n = E_n\psi_n, \quad n = 1, 2, \dots \qquad E_n \text{ real} \tag{2.2}$$ {?}

for simplicity let us assume everything is discrete while E_n are all real because of the hermiticity of the Hamiltonian and in general one has to express ψ as a linear combination of the basis elements and for each element has to add a time dependent exponential factor

$$\psi = \sum_n c_n\psi_n \to \psi(t) = \sum_n c_n e^{-iE_nt/\hbar}\psi_n. \tag{2.3}$$ {?}

In principal this procedure is easy and really straightforward:

$$\mathcal{H}(t)\psi_n(t) = E_n\psi_n(t), \quad n = 1, 2, \dots \qquad E_n \text{ real} \tag{2.4}$$ {?}

where we have implicitly supposed the E_n to be non degenerate and constant in time. ψ_n are called the stationary states of the system and of course the ψ_n form a complete set of orthonormal vector basis

$$\sum_n |\psi_n\rangle \langle\psi_n| = \mathbb{1} \tag{2.5}$$ {?}

$$(\psi_n, \psi_k) = \delta_{nk} \tag{2.6}$$ {?}

but each ψ_j is defined up to an independent phase factor.

Let us now discuss the case of a time dependent Hamiltonian; at each time where have to use the Hamiltonian evaluated at that time, so generalizing what written above

$$\mathcal{H}(t)\psi(t)_n = E_n(t)\psi_n(t), \quad n = 1, 2, \dots \qquad E_n(t) \text{ real} \tag{2.7}$$ {?}

and as the Hamiltonian changes in time, then its eigenvalues do. Of course at each time the eigenvalues form again a complete orthonormal set. This is, in principle, available to us.

Remark 1. We stress again the fact that each eigenfunction is determined up to a phase. This factor can be both dependent on time and on n.

Now, there is no hope to recover the exact solution, even though you have solved the eigenvalue problem for each time. What we can do is to use eq.(2.1) for rewriting $\psi(t)$ as

$$\psi(t) = \sum_n c_n(t)e^{-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'}\psi_n(t) \tag{2.8}$$?eq:2.4?

and it will reduce to (2.1) in the case of time independence. So what we will get is

$$i\hbar\sum_n \left(\dot{c_n}(t)\psi_n(t) - \frac{i}{\hbar}c_n(t)E_n(t)\psi_n(t) + c_n(t)\dot{\psi_n}(t)\right) e^{-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'} \tag{2.9}$$ {?}

$$= c_n(t)E_n(t)\psi_n(t)e^{-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'} \tag{2.10}$$ {?}

so, erasing the equal terms, we obtain

$$\sum_n \left(\dot{c_n}(t)\psi_n(t) - \frac{i}{\hbar} c_n(t) E_n(t)\psi_n(t) + c_n(t)\dot{\psi_n}(t) \right) e^{-\frac{i}{\hbar}\int_0^t E_n(t')\,dt'} = 0. \tag{2.11}$$?eq:2.5?

and now we take the scalar product with the vector $\psi_k(t)$

$$\dot{c}_n = -\sum_n c_n(t) e^{-\frac{i}{\hbar}\int_0^t (E_k(t') - E_n(t'))\,dt'} \left(\psi_k(t), \dot{\psi}_n(t) \right) \qquad \forall k \tag{2.12}$$ {?}

Remark 2. The last equation is exact! There are no approximations involved so far!

Let's focus for the moment on the term $\left(\psi_k(t), \dot{\psi}_n(t) \right)$

$$\mathcal{H}(t)\psi(t)_n = E_n(t)\psi_n(t), \quad n = 1, 2, \dots \tag{2.13}$$ {?}

and we differentiate with respect to time on both sides

$$\frac{\partial}{\partial t}\mathcal{H}(t)\psi_n(t) + \mathcal{H}(t)\dot{\psi}_n(t) = \frac{\partial}{\partial t} E_n(t)\psi_n(t) + E_n(t)\dot{\psi}_n(t) \tag{2.14}$$ {?}

and again we take again the scalar product with a generic state $\psi_k(t)$

$$\left(\psi_k(t), \frac{\partial \mathcal{H}(t)}{\partial t}\psi_n(t) \right) + E_k(t) \left(\psi_k(t), \dot{\psi}_n(t) \right) = \dot{E}_n(t)\delta_{nk} + E_n \left(\psi_k(t), \dot{\psi}_n(t) \right) \tag{2.15}$$ {?}

so it is appropriate to collect some terms, creating an energy difference, obtaining

$$(E_n(t) - E_k(t)) \left(\psi_k(t), \dot{\psi}_n(t) \right) = -\dot{E}_n(t)\delta_{nk} + \left(\psi_k(t), \frac{\partial \mathcal{H}(t)}{\partial t}\psi_n(t) \right) \tag{2.16}$$ {?}

and the previous result is true in general! There are no approximations involved at all!

If we restrict ourselves at the specific case $k = n$

$$\dot{E_(t)} = \left(\psi_k(t), \frac{\partial \mathcal{H}(t)}{\partial t}\psi_n(t) \right) \tag{2.17}$$ {?}

while in the case $k \neq n$ we can straightforwardly derive from the eigenvalue problem [2]

$$\left(\psi_k(t), \dot{\psi}_n(t) \right) = \frac{\left(\psi_k(t), \frac{\partial \mathcal{H}(t)}{\partial t}\psi_n(t) \right)}{(E_n(t) - E_k(t))} \tag{2.18}$$ {?}

So we found an explicit expression relating the relative energy gap in time, the time derivative of the Hamiltonian and the scalar product of the time derivative of the wavefunction with any other wavefunction. We remark that each time dependent wavefunction $\psi_n(t)$ is defined up to a phase factor that can depend on n and may depend on time. With this freedom we are left all alone.

So from now on we agree to restrict the phase factor to be for each n such that

$$\left(\psi_k(t), \dot{\psi}_n(t) \right) = 0, \qquad \forall n \tag{2.19}$$ eq:requirement

[2] Remember that we assumed non degeneracy in energy spectrum in all the time

Remark 3. Making use of the requirement (2.19), the phase freedom is eliminated. Once we chose a phase factor at time $t = 0$ for $\psi_n(0)$, no more flexibility is left.

$$\dot{c}_k(t) = -\sum_{n\neq k} c_n(t) e^{i\int_0^t \omega_{kn}(t')\,dt'} \left(\psi_k(t), \dot{\psi}_n(t)\right) \tag{2.20}$$ {?}

$$= \sum_{n\neq k} \frac{c_n(t)}{\hbar\omega_{nk}(t)} e^{i\int_0^t \omega_{kn}(t')\,dt'} \left(\psi_k(t), \frac{\partial\mathcal{H}(t)}{\partial t}\psi_n(t)\right) \qquad \forall k \tag{2.21}$$ eq:2.11

where we defined $\omega_{nk}(t) = \frac{E_k(t)-E_n(t)}{\hbar}$.

Remark 4. We stress again that Eq.(2.21) is obtain manipulating the Schrödinger equation only letting the Hamiltonian to vary in time.

2.1.1 Adiabatic condition

Now we go to the *adiabatic situation*. The so called *Adiabatic condition* is a result mainly due to Born&Fock in 1928 Born (1928)

The main assumption we'll do is that the Hamiltonian we're considering is a slowly varying operator, that is to say

$$\frac{\partial\mathcal{H}}{\partial t}(t) \text{ is "small"} \tag{2.22}$$ {?}

The term "small" will be quantitatively clear later on while, physically, it's reasonable to say that the quantities $\psi_n(t), E_n(t)$ and $c_n(t)$ are expected to slowly change in time.

Let's then continue with the original work of Fock and Born, back to 1928: suppose to have as initial solution $\psi(0) = \psi_n(0)$, that is to say that the original initial state is equal to a particular eigenvector of the Hamiltonian at time $t = 0$. So we have $c_k(0) = \delta_{kn}$(the same chosen in (**??**))

Notice that our reasoning is perfectly consistent in the framework of the first order perturbation theory; since the term $\frac{\partial\mathcal{H}}{\partial t}$ is explicitly appearing in (2.21), we can expand the equation and ignore all the upper degree terms, we have that for $k \neq n$,

$$\dot{c}_n(t) \simeq \frac{1}{\hbar\omega_{kn}} e^{i\omega_{kn}t} \left(\psi_k, \frac{\partial\mathcal{H}}{\partial t}(t)\psi_n\right) \tag{2.23}$$ {?}

while for the n-th term we have $c_n(t) \simeq 1$: it starts at 1 and stay fixed for all times. The $\dot{c}_n(t)$ can be instead integrated and

$$c_n(t) \simeq -\frac{1}{\hbar\omega_{kn}^2} \left(e^{i\omega_{kn}t} - 1\right) \left(\psi_k, \frac{\partial\mathcal{H}}{\partial t}(t)\psi_n\right) \tag{2.24}$$ {?}

and so, while the term c_n remains close to 1, all the other terms, despite the fact that they start from zero, they change significantly in the way explicited above.

So,once is provided that the condition

$$\frac{1}{\omega_{kn}} \left|\left(\psi_k, \frac{\partial\mathcal{H}}{\partial t}(t)\psi_n\right)\right| \ll \hbar\omega_{kn}, \qquad \forall k \neq n \tag{2.25}$$ eq:2.14

is satisfied, then

$$\psi(t) \simeq e^{-\frac{i}{\hbar}\int_0^{t'} E_n(t)\,dt}\psi_n(t) \tag{2.26}$$ {?}

and this closes the statement of the adiabatic theorem of quantum mechanics.

Remark 5. Eq.(2.25) is the quantitative statement of what we mean by "adiabatic condition".

And now comes the step taken by Berry; suppose $\mathcal{H}(t)$ is cyclic, that is, $\mathcal{H}(0) = \mathcal{H}(T)$ for some T[3].

Question: How behaves the approximate solution? Are they cyclic in a similar sense?

Answer: the solution must be cyclic in some sense. Because of the non degeneracy and no crossing levels, we have that the eigenvalues of $\mathcal{H}(T)$ are the same of $\mathcal{H}(0)$

$$E_n(T) = E_n(0) \tag{2.27}$$ {?}

$$\psi(0) = \psi_n(0) \quad \Rightarrow \quad \psi(T) \simeq e^{-\frac{i}{\hbar}\int_0^{T} E_n(t)\,dt}\psi_n(T) \tag{2.28}$$ {?}

by the Adiabatic Theorem. And now we ask: is this a cyclic solution? The answer is still **yes** but we have $\psi(T) = \psi(0)$ apart from a phase, i.e.,

$$\psi(T) = \text{(n-dependent phse)}\psi_n(0) \tag{2.29}$$ {?}

It follows then the following equalities:[4].

$$\psi_n(T) = e^{i\varphi^{(n)}_{geom}}\psi_n(0) \tag{2.30}$$ eq:geometric_ph

$$\psi(T) \simeq e^{i\varphi^{(n)}_{tot}}\psi(0) \qquad i.e., \qquad \varphi^{(n)}_{tot} = \arg\left(\psi(0), \psi(T)\right) \tag{2.31}$$ eq:total_phase

$$\varphi^{(n)}_{tot} = \varphi^{(n)}_{geom} + \varphi^{(n)}_{dyn} \qquad i.e. \qquad \varphi^{(n)}_{geom} = \varphi^{(n)}_{tot} - \varphi^{(n)}_{dyn} \tag{2.32}$$ eq:Berry_discov

where we defined

$$\varphi^{(n)}_{dyn} = \frac{i}{\hbar}\int_0^T E_n(t)\,dt \tag{2.33}$$ {?}

So, in the end, this is the original work of Berry presented in a slightly different language.

Remark 6. Eq. (2.32) is regarded as the original discovery of Berry. Eq(2.31) is the definition of φ_{tot}; it is something we defined using the result of the Adiabatic Theorem: if there are no degeneracies andd no crossing levels, then every approximate solution given by the adiabatic condition will also be cyclic. (2.30) instead defines how every phase of every wavefunction evolves in time provided that condition (2.19) is satisfied. We recall that (2.19) is only a convention: given the general expression for $(\psi_k, \dot{\psi}_n)$ in the particular case $k = n$, there's no way for controlling the generic phase between those two, but if (2.19) is satisfied, then a formula like (2.30) must exist.

Remark 7. One could argue that changing the convention (2.19) then the definition for (2.30) must change. This is absolutely reasonable, but nonetheless we will see that the geometric phase will not change under different assumptions: this invariance is one of the most important properties of the Berry Phase.

[3] Cyclic condition on the Hamiltonian

[4] They're all approximate in the sense of the adiabatic theorem, but we put the equality sign with no confusion

2.2 Berry original derivation with parameter space

We want no to present the work performed by Berry in his original work in 1983 in the spirit of the parameter space.

The original assumption was that the Hamiltonian, apart from being hermitian, depends on a set of external parameters, let's say $\underline{\mathrm{R}}$, that is $\mathcal{H} \equiv \mathcal{H}(\underline{\mathrm{R}})$ with $\underline{\mathrm{R}}$ belonging to a multidimensional real parameter space. Then Berry imagined the following situation: suppose the external classical environment is slowly changing in time, like when we put a spin $\frac{1}{2}$ particle in a magnetic field and we slowly change the external magnetic field. Imagine then the real parameter space being slowly dependent in time, that is to say, $\underline{\mathrm{R}}$ itself to be time dependent, so that the Hamiltonian si explicitly time dependent $\mathcal{H}(\underline{\mathrm{R}}(t))$. The parameter now that varies adiabatically is of course now $\underline{\mathrm{R}}(t)$.

Remark 8. We recall that $\underline{\mathrm{R}}(t)$ is a set of real independent parameters and thanks to the Adiabatic condition the quantity $\frac{\partial \underline{\mathrm{R}}}{\partial t}$ is small.

$$\mathcal{C} = \{\underline{\mathrm{R}}(t) \mid 0 \leq t \leq T\} \tag{2.34}$$ eq:Curve

Figure missing! Place here as soon as possible!

The curve $\mathcal{C}$ is the curve traced by $\underline{\mathrm{R}}(t)$ letting t varying. $\mathcal{C}$ is of course cyclic. The curve $\mathcal{C}$ is then our domain of interest and for each point in $\mathcal{C}$ we have an associated Hamiltonian.

$$\mathcal{H}(t)\,|n;\underline{\mathrm{R}}\rangle = E_n(\underline{\mathrm{R}})\,|n;\underline{\mathrm{R}}\rangle \tag{2.35}$$ {?}

$$\langle n';\underline{\mathrm{R}}\,|\,n;\underline{\mathrm{R}}\rangle = \delta_{n'n} \tag{2.36}$$ {?}

and we have of course an orthonormal basis at each point of the multidimensional parameters space.

Remark 9. To be precise, we should refer to the eigenvalues $E_n(\underline{\mathrm{R}})$ not as eigenvalues of the Hamiltonian but as *eigenvalues of the Hamiltonian at a certain point $\underline{\mathrm{R}}$ of the parameter space*. We recall moreover that each wavefunction $|n;\underline{\mathrm{R}}\rangle$ is defined up to a phase factor that may depend on n and on $\underline{\mathrm{R}}$.

Remark 10. Thanks to the non degeneracy of the eigenvalues of the Hamiltonian, we have no ambiguity in defining the eigenvectors of the Hamiltonian, that is to say, there are not crossing levels of energy. Let's say for example that we start from the point $\underline{\mathrm{R}}(0)$ in tha parameter space, then we can recover a set of well defined single valued wavefunctions for the Hamiltonian $\mathcal{H}(\underline{\mathrm{R}}(0))$. Letting now t varying from 0 to T we have a complete set of well defined single valued vawefunctions for every point and when $t = T$ we have the same set of eigenfunctions as we had in $t = 0$. Each eigenfucntion remains, anyway, defined up to an arbitrary phase.

At this stage Berry recover the Adiabatic Theorem and tries to solve the classical Schrödinger equation in the case in which the initial state is the n-th eigenstate of the Hamiltonian at $t = 0$:

$$\begin{cases} i\hbar\dot{\psi}(t) = \mathcal{H}(\underline{\mathrm{R}}(t))\psi(t) \\ \psi(0) = |0;\underline{\mathrm{R}}(0)\rangle \end{cases} \tag{2.37}$$ {?}

which, for intermediate times, within the validity of the Adiabatic Theorem, gives the solution

$$\psi(t) \simeq e^{-\frac{i}{\hbar}\int_0^t E_n(\underline{\mathrm{R}}(t'))\,dt' + \gamma_n(t)}\,|n;\underline{\mathrm{R}}(t)\rangle \tag{2.38}$$ eq:gen_s

and we easily see that $\gamma_n(0) = 0$, since it has to match with the initial condition.

The first term in the exponential of eq.(2.38) is the *dynamical phase* while the term $\gamma_n(t)$ is the geometric phase. This latter phase is non integrable and so far we are not ready to handle it.

So the next step to take is to take the (general) solution (2.38), to plug it into the Schrödinger equation itself and try to extract an equation for $\gamma_n(t)$.

Remark 11. The set $|n;\underline{\mathrm{R}}\rangle$ form a set of single-valued eigenvectors in the parameter space. Pay attention that this condition is the crucial difference in spirit with the derivation given in the previous section. There the original assumption was to put $\left(\psi_n(t), \dot{\psi}_n(t)\right)$ in order to eliminate any arbitrary freedom on the choice of the initial wavefunction.

Remark 12. What Berry did is the following: he applied the Adiabatic Theorem and obtained an approximated solution for $\psi(t)$. He then put $\psi(t)$ itself into the Schrödinger Equation and derived an equation of motion for $\gamma_n(t)$

So, putting eq.(2.38) into the Schrödinger equation, is equivalent to write (as a consequence of the Adiabatic Theorem)

$$\dot{\gamma}_n(t)\,|n;\underline{\mathrm{R}}(t)\rangle \simeq i\frac{d}{dt}\,|n,\underline{\mathrm{R}}(t)\rangle \tag{2.39}$$ {?}

and then sandwiching with a Ket,

$$\dot{\gamma}_n(t) \simeq i\,\langle n;\underline{\mathrm{R}}(t)|\,\frac{d}{dt}\,|n:\underline{\mathrm{R}}(t)\rangle \tag{2.40}$$ {?}

$$= i\,\langle n;\underline{\mathrm{R}}(t)|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}(t)\rangle\,\dot{\underline{\mathrm{R}}}(t)^5 \tag{2.41}$$ {?}

Remark 13. We notice that the result

$$\dot{\gamma}_n(t) \simeq i\,\langle n;\underline{\mathrm{R}}(t)|\,\frac{d}{dt}\,|n:\underline{\mathrm{R}}(t)\rangle \tag{2.42}$$ {?}

is a consequence of the Schrödinger Equation and not a condition imposed on the system.

Remark 14. We have $|n;\underline{\mathrm{R}}(0)\rangle = |n;\underline{\mathrm{R}}(T)\rangle$ since they're globally well defined.

Performing the circuitation along the curve $\mathcal{C}$ defined in (2.34), we have

$$\gamma_n(T) \equiv \gamma_n(0) = i\oint_{\mathcal{C}} \langle n;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle\,\dot{\underline{\mathrm{R}}}(t)\,dt = i\oint_{\mathcal{C}} \langle n;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle\cdot d\underline{\mathrm{R}} \tag{2.43}$$ eq:2.26

and this is exactly what we wrote above.

In the end, we see that

$$\langle n;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle = i\Im\,\langle n;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle \tag{2.44}$$ eq:2.27

and so plugging (2.44) into (2.43) we obtain

$$\gamma_n(\mathcal{C}) = -\Im\oint \langle n;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle\cdot d\underline{\mathrm{R}} \tag{2.45}$$ {?}

$$= -\Im\iint_{\mathcal{S}} \nabla\wedge\langle n;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle\cdot d\mathcal{S}^6 \tag{2.46}$$ {?}

$$= -\Im\iint_{\mathcal{S}} \left(\underline{\nabla}\,\langle n;\underline{\mathrm{R}}|\right)\wedge\left(\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle\right)\cdot d\mathcal{S} \tag{2.47}$$ {?}

$$= -\Im\iint_{\mathcal{S}} \left(\sum_{m\neq n}\underline{\nabla}\,\langle n;\underline{\mathrm{R}}|\right)|m;\underline{\mathrm{R}}\rangle\wedge\langle m;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle \tag{2.48}$$ {?}

and the term $m = n$ is neglected since gives a zero contribution: a pure imaginary term times a pure imaginary term gives an only real contribution, so neglected by the operator $\Im$.

Then from $\mathcal{H}(\underline{\mathrm{R}})\,|n;\underline{\mathrm{R}}\rangle = E_n(\underline{\mathrm{R}})\,|n;\underline{\mathrm{R}}\rangle$, applying the gradient operator on both sides, we obtain for $m \neq n$

$$\langle m;\underline{\mathrm{R}}|\,\underline{\nabla}\,|n;\underline{\mathrm{R}}\rangle = \frac{\langle m;\underline{\mathrm{R}}|\,\underline{\nabla}\mathcal{H}(\underline{\mathrm{R}})\,|n;\underline{\mathrm{R}}\rangle}{E_n(\underline{\mathrm{R}}) - E_m(\underline{\mathrm{R}})}. \tag{2.49}$$ {?}

The final result is then

$$\gamma_n(\mathcal{C}) = -\iint_{\mathcal{S}} V_n(\underline{\mathrm{R}}) \cdot d\mathcal{S} \tag{2.50}$$ {?}

where we defined V_n as

$$V_n(\underline{\mathrm{R}}) := \Im \sum_{m\neq n} \frac{\langle n;\underline{\mathrm{R}}|\,\underline{\nabla}\mathcal{H}(\underline{\mathrm{R}})\,|m;\underline{\mathrm{R}}\rangle \wedge \langle m;\underline{\mathrm{R}}|\,\underline{\nabla}\mathcal{H}(\underline{\mathrm{R}})\,|n;\underline{\mathrm{R}}\rangle}{\left(E_n(\underline{\mathrm{R}}) - E_m(\underline{\mathrm{R}})\right)^2} \tag{2.51}$$ eq:2.31

Remark 15. Berry's comment at this stage is that the result does not depend on $\underline{\mathrm{R}}$ since the gradient is only acting on $\mathcal{H}(\underline{\mathrm{R}})$, so it is independent on the choice of the phase of the wavefunction. The final take at home message is then that the geometric phase $\gamma_n(\mathcal{C})$ does not depend on the particular choice of the phase of the eigenvector $|n;\underline{\mathrm{R}}\rangle$ of the Hamiltonian at each point of the parameter space, under the assumption that *the eigenvectors are globally well defined.*

⟨rem:freedom⟩

Remark 15 leads to an enormous amount of freedom in the choice of the global phase $\chi(\underline{\mathrm{R}})$

$$|n;\underline{\mathrm{R}}\rangle \to e^{i\chi(\underline{\mathrm{R}})}\,|n;\underline{\mathrm{R}}\rangle \tag{2.52}$$ {?}

2.2.1 Two fold degeneracies

Let us suppose that we are in the proximity of a two fold degeneracy. By degeneracy we mean that two levels of the Hamiltonian happen to be degenerate of a certain point of the phase space.

We can suppose in $\underline{\mathrm{R}} = 0$ we have a degeneracy for the Hamiltonian. So if we are far from zero, we have o problems at all, but if we are close to 0, we have to work in a different way. The two crossing levels are the most important, so from a Quantum Mechanical point of view, the problem is only a two level problem.

$$\mathcal{H}(\underline{0}) = 0; \qquad \mathcal{H}(\underline{\mathrm{R}}) = |\pm;\underline{\mathrm{R}}\rangle = E_\pm(\underline{\mathrm{R}}) = |\pm;\underline{\mathrm{R}}\rangle \tag{2.53}$$ {?}

$$E_+(\underline{\mathrm{R}}) > E_-(\underline{\mathrm{R}}), \qquad \underline{\mathrm{R}} \neq 0 \tag{2.54}$$ {?}

$$E_+(\underline{0}) = E_-(\underline{0}) = 0. \tag{2.55}$$ {?}

So, now, without any loss of generality, we can make use of the Pauli Matrices for defining the Hamiltonian to be in the following way

$$\mathcal{H}(\underline{\mathrm{R}}) = \frac{1}{2}; \qquad E_\pm(\underline{\mathrm{R}}) = \pm\frac{1}{2}R, \qquad R = |\underline{\mathrm{R}}| \tag{2.56}$$ {?}

$$|+;\underline{\mathrm{R}}\rangle\,\langle +;\underline{\mathrm{R}}| = \frac{1}{2}\left(1 \pm \hat{R}\cdot\underline{\sigma}\right) \tag{2.57}$$ eq:2.33

[6] Following Berry's argument, we are now restricting ourselves in the case in which the parameter space is a 3D space, so the simplest form of Stoke's Theorem can be applied.

And so we have to plug (2.57) into (2.51): the summation becomes an only single term and, recognizing that $E_n(0) - E_m(0) = +\frac{1}{2}R - (-\frac{1}{2}R)$, we obtain

$$\underline{V}_+(\underline{\mathrm{R}}) = \frac{R_j}{2R^3} \tag{2.58}$$ eq:2.35

So now comes the result of Berry: the phase gained by the wavefunction is exactly given by the integration of (2.58) and is the solid angle shifted by the curve $\mathcal{C}$. Berry refereed to this result as the *magnetic field of a "magnetic monopole"*

$$\gamma_+(\mathcal{C}) = -\frac{1}{2}\Omega\left[\mathcal{C}\right], \qquad \Omega\left[\mathcal{C}\right] = \text{solid angle at } \underline{0} \tag{2.59}$$ {?}

3 Aharonov-Anandan and Samuel-Bhandari generalizations

3.1 Aharonov-Anandan generalization (1987)

The first relaxation was taken in Aharonov and Anandan (1987) where the authors considered the Adiabatic Hypothesis: they showed that the latter is not needed in order to get a geometric effect.

Let us take a t-dependent Hamiltonian

$$i\hbar\frac{d}{dt}\psi(t) = \mathcal{H}(t)\psi(t) \tag{3.1}$$ {?}

and assume that we found a solution for the problem that is cyclic in the sense given in the previous chapter, that is,

$$\psi(T) = e^{i\psi_{tot}}\psi(0) \tag{3.2}$$ eq:3.1

No assumptions on the cyclicity of the Hamiltonian is assumed in (3.2), nor no assumption on the adiabaticity of the Hamiltonian has been made neither and we also don't need the fact that $\mathcal{H}(T) = \mathcal{H}(0)$, but if we have a periodicity on the solution we can associate to the wavefunction a new concept of geometric phase[1]:

$$\varphi_{geom} = \varphi_{tot} - \varphi_{dyn} \tag{3.3}$$ {?}

where

$$\varphi_{dyn} = -\frac{i}{\hbar}\int_0^T \langle\psi(t)|\,\mathcal{H}(t)\,|\psi(t)\rangle\,dt \tag{3.4}$$ eq:phi_dyn

Before exploit extensively the result achieved by Aharonov and Anandan, we can summarize them briefly:

1. **Clear definition of geometric phase**: under the condition of cyclicity of the solution $\psi(t)$, it is possible to derive the quantity φ_{tot}. Then, given the prescription for the definition of a dynamical phase, Eq. (3.4), is possible to derive the geometric phase understood as a difference between two terms. In particular, in the case of an adiabatic condition for the Hamiltonian, the calculation reduces to the ones already performed by Berry.
2. **The geometric phase depends only on the projection on the ray space**: it is not anymore important the wavefunction itself but it is only important the movement of the trace of the solution projected on the space of density matrices. Being a pure

[1] from now on we'll distinguish the Berry phase from the present geometric phase since the concept we're dealing right now is quite different form the initial idea given by Berry: the concept of cyclicity and adiabaticity are now not needed.

state, well defined, single valued unitary vector in Hilbert space for each time, $\psi(t)$ can be uniquely determined by the corresponding 1 dimensional projection operator, or, as we will call it, *a point in the ray space*. In a certain sense, Berry already stated this result, but the A-A were able to state this result in a more general perspective, stating that the geometric phase lives in the ray space.

3. **The parameter space concept is not needed to arrive to tha concept og geometric phase**: we're not required to know the Hamiltonian acquire its dependence on the $\underline{R}$vector.

3.2 First Mathematical Interlude

$$\mathfrak{B} = \{\psi \in \mathscr{H} : \ \langle \psi, \psi \rangle = 1\} \subset \mathscr{H} \tag{3.5}$$ {?}

We notice immediately that $\mathfrak{B}$ is not a linear vector space. We define therefore the transformation

$$\psi \in \mathfrak{B} \Rightarrow \psi' = e^{i\alpha}\psi \in \mathfrak{B}, \qquad 0 \leq \alpha \leq 2\pi \tag{3.6}$$ {?}

The idea is that two vectors that differ only by a phase factor should be regarded as equivalent. We can also define now the equivalence class by fixing ψ and letting α varying:

$$\mathcal{R} := \left\{\rho(\psi) = |\psi\rangle \langle\psi| \ \text{ or } \psi^\dagger\psi | \psi \in \mathfrak{B}\right\}. \tag{3.7}$$ {?}

We will call $\mathcal{R}$ *real space*, while ρ is the well known projective operator. We notice that if we denote by N the dimension of the Hilbert space $\mathscr{H}$, then we have that $\dim(\mathcal{R})$ has $2(N-1)$ real dimensions (or equivalently $N-1$ complex dimensions). We define as well the inverse of the projection operator, the operator π, in the following way:

$$\pi : \mathfrak{B} \to \mathcal{R} \qquad : \qquad \psi \in \mathfrak{B} \to \rho(\psi) = \psi^\dagger\psi \in \mathcal{R} \tag{3.8}$$ {?}

and goes into CP^{N-1}.

Points in the real space are in $1-1$ correspondence with the pure real state of the system. The mathematical description is

$$\rho(\psi) \in \mathcal{R} \to \pi^{-1}(\rho(\psi)) := \left\{\psi' = e^{i\alpha}\psi \in \mathfrak{B} | \psi \text{ fixed }, 0 \leq \alpha \leq 2\pi\right\} \subset \mathfrak{B} \tag{3.9}$$ {?}

We now consider curves on the space $\mathfrak{B}$. Given a curve

$$\mathcal{C} := \{\psi(s) \in \mathfrak{B} | s_1 \leq s \leq s_2\} \subset \mathfrak{B} \tag{3.10}$$ {?}

we consider its projection into the real space $\mathcal{R}$ through π into the set

$$C = \pi\left[\mathcal{C}\right] = \left\{\rho(\psi(s)) = \psi(s)\psi^\dagger(s) \in \mathcal{R} | s_1 \leq s \leq s_2\right\}. \tag{3.11}$$ {?}

So for our purposes the most general curve will be

$$\mathcal{C}' = \left\{\psi'(s) = e^{i\alpha(s)}\psi(s) | \psi(s) \in \mathcal{C}, s_1 \leq s \leq s_2\right\}, \tag{3.12}$$ {?}

that denotes all the possible lifts of the original projected curve. Now comes natural to define the tangent vector

$$u(s) = \frac{d}{ds}\psi(s) = \dot{\psi}(s) \tag{3.13}$$ {?}

$$(\psi(s), \dot{\psi}(s)) = \Im(\psi(s), u(s)) \tag{3.14}$$ eq:3.12

$$u'(s) = e^{i\alpha(s)}(u(s) + i\dot{\alpha}(s)\psi(s)) \tag{3.15}$$ {?}

$$u_\perp(s) = u(s) - \psi(s)(\psi(s), u(s)) = u'_\perp(s) = e^{i\alpha(s)}u_\perp(s) \tag{3.16}$$ {?}

$$\mathcal{L}[\mathcal{C}] = \int_{s_1}^{s_2} (u_\perp(s), u_\perp(s))^{1/2} \cdot ds \tag{3.17}$$ {?}

$$= \int_{s_1}^{s_2} \left\{ \left(\dot{\psi}(s), \dot{\psi}(s)\right) - \left(\psi(s), \dot{\psi}(s)\right) - \left(\dot{\psi}(s), \psi(s)\right) \right\}^{1/2} ds \tag{3.18}$$ {?}

i $\rho_1 = \rho(\psi_1), \rho_2 = \rho(\psi_2)$; then $\mathrm{Tr}(\rho_1\rho_2) > 0$, i.e., $|(\psi_1, \psi_2)| \neq 0$, then exists an unique geodesic $\mathcal{C}_0$

ii $\psi_1 \in \pi^{-1}(\rho_1), \psi_2 \in \pi^{-1}(\rho_2)$

$$(\psi_1, \psi_2) = \cos\theta, \qquad 0 \leq \theta \leq \pi(\alpha) \tag{3.19}$$ {?}

In general the inner product between two complex quantities gives a complex quantity. If they're real and positive definite, they're said to be in phase one each other in the Plancherel sense.

iii If we consider the geodesic $\mathcal{C}_0$ from ρ_1 to ρ_2 and then we take the lift

$$\mathcal{C}_0 = \left\{ \psi_0(s) = \psi_1 \cos(s) + (\psi_2 - \psi_1 \cos\theta)\frac{\sin s}{\sin\theta} \mid 0 \leq s \leq \theta \right\} \subset \mathfrak{B} \tag{3.20}$$ {?}

$$\dot{\psi}_0(s) = u_0(s) = -\psi_1 \sin s + (\psi_2 - \psi_1 \cos\theta)\frac{\cos s}{\sin\theta} \tag{3.21}$$ {?}

$$(u_0(s), u_0(s)) = 1, \qquad (\psi_0(s), u_0(s)) = 0, \tag{3.22}$$ {?}

$$u_\perp(s) = u_0(s), \qquad \pi[\mathcal{C}_0] = \mathcal{C}_0 \tag{3.23}$$ {?}

$$\mathcal{L}[\pi[\mathcal{C}_0]] = \theta \tag{3.24}$$ {?}

Now we want to introsuce another geometrical object:

$$\mathcal{A} = \text{one-form on } \mathcal{B} = -i\psi^\dagger\, d\psi \tag{3.25}$$ {?}

On every $\mathcal{C} \subset \mathfrak{B}$ (recalling equation (3.14))

$$i\int_{s_1}^{s_2} \left(\psi(s), \frac{d}{ds}\psi(s)\right) ds = \Im \int_{s_1}^{s_2} (\psi(s), u(s))\, ds \tag{3.26}$$ {?}

and the last integral does not depend on how we parametrize it; it's a geometric object. In the language og differential geometry it is

$$\int_{\mathcal{C}_0} \mathcal{A} \tag{3.27}$$ {?}

and its integral along any curve is the dynamical phase.

3.3 S-R generalization (1988)

cyclic condition is also not needed for achieving a geometric phase

$$\mathcal{C}_{\prime} = \text{geodesic in } \mathcal{R} \Rightarrow \mathcal{C}_{\prime} = \text{special lift of } \mathcal{C}_0 \text{ to } \mathfrak{B} \tag{3.28}$$ {?}

$$\Rightarrow \mathcal{C} = \text{general lift of } \mathcal{C}_0 \text{ to } \mathfrak{B} \tag{3.29}$$ {?}

$$\int_{\mathcal{C}_0} \mathcal{A} = \Im \int_0^{\theta} (\psi(s), u(s)\, dS = \arg(\psi(0), \psi(\theta)) \tag{3.30}$$ {?}

So how's they did: take the hermitian Hamiltonian $\mathcal{H}$

$$i\hbar \frac{d}{dt}\psi(t) = \mathcal{H}(t)\psi(t) \tag{3.31}$$ {?}

and now consider the set of points

$$\{0 \leq t \leq T \colon \psi(t) \text{ is a solution}\} \equiv \mathcal{C}_0 \subset \mathfrak{B} \tag{3.32}$$ {?}

$$\varphi_{geom}\,[\text{Energetic Schrödinger equation}] = \oint_{\mathcal{C}_0} \mathcal{A}. \tag{3.33}$$ {?}

This is the tool in order to relax the assumption of the cyclic Hamiltonian.

4 The kinematic approach and the Bargmann's Invariant

$$\mathcal{C} \to \mathcal{C}' = \left\{ \psi'(s') = \psi(s) \mid s' = f(s), \frac{\partial df(s)}{\partial ds} \geq 0 \right\} \tag{4.1}$$ {?}

The key idea is to look at all the possible transformations that we can apply to the initial curves preserving the reparametrization invariance and the gauge invariance

$$\varphi_{geom}\left[\mathcal{C}\right] = \varphi_{tot}\left[\mathcal{C}\right] - \varphi_{dyn}\left[\mathcal{C}\right] \tag{4.2}$$ eq:parametrizat

$$\varphi_{tot}\left[\mathcal{C}\right] = \arg(\psi(s_1), \psi(s_2) \tag{4.3}$$ {?}

$$\varphi_{dyn}\left[\mathcal{C}\right] = \Im \int_{s_1}^{s_2} \left(\psi(s), \frac{\partial d\psi(s)}{\partial ds}\right) ds = -i \int_{s_1}^{s_2} \left(\psi(s), \frac{\partial d\psi(s)}{\partial ds}\right) ds = \int_{\mathcal{C}} \mathcal{A}\, ds \tag{4.4}$$ {?}

And the quantity in (4.2) needs to be reparametrization invariant and gauge invariant.

$$\varphi_{geom}\left[\text{any geometric in } \mathcal{R}\right] = 0. \tag{4.5}$$ {?}

4.1 Bargmann's Invariant

$$\psi_j, \quad j = 1, 2, 3, \in \mathfrak{B} \tag{4.6}$$ {?}

$$\Delta_3\left(\psi_1, \psi_2, \psi_3\right) = \left(\psi_1, \psi_2\right)\left(\psi_2, \psi_3\right)\left(\psi_3, \psi_1\right) \tag{4.7}$$ {?}

$$= \mathrm{Tr}(\rho_1 \rho_2 \rho_3) \tag{4.8}$$ {?}

Where by $\rho_i, i = 1, 2, 3$ we denoted the density matrices and we recall that their product is a ray space quantity.

So in general the phase of the Bargmann quantity can be shown to be a geometric phase

$$\arg(\Delta_3\left(\psi_1, \psi_2, \psi_3\right)) = \arg(\psi_1, \psi_2) + \arg(\psi_2, \psi_3) + \arg(\psi_3, \psi_1) \tag{4.9}$$ {?}

$$= \varphi_{dyn}\left[\mathcal{C}_{12}\right] + \varphi_{dyn}\left[\mathcal{C}_{23}\right] + \varphi_{dyn}\left[\mathcal{C}_{31}\right] \tag{4.10}$$ {?}

$$= \varphi_{dyn}\left[\mathcal{C}_{12} \cup \mathcal{C}_{23} \cup \mathcal{C}_{31}\right] \tag{4.11}$$ {?}

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