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Aspects of Quantum Mechanics: Quantum Correlations and Geometric Phase

2.1 Quantum correlations

The various predictions of quantum mechanics have been successfully verified in numerous experiments. However, the theory presents a non-realistic description of nature, in the sense that the measurement of a physical quantity does not reveal a pre-existing or pre-determined value. The theory does not predict the outcome of any measurement with complete certainty, rather it indicates probabilities of outcomes with the indeterminism of observable quantities constrained by the uncertainty principle. According to this principle, if two physical quantities are described by non-commuting operators than the knowledge of any one of them precludes the knowledge of the other. In 1935, Einstein and his two collaborators B. Podolsky and N. Rosen (EPR) pointed out in their paper [99] that in situations involving specially-prepared pairs of particles, this orthodox principle conflicted with locality. EPR argued that if non-local influences are forbidden, and if quantum theoretical predictions are correct, then the measurements (whose outcomes are correlated) must reveal pre-existing values. Hence, EPR claimed that quantum mechanics, cannot be considered a complete theory of physical reality since it denies the existence of any such pre-existing values. They stated in their paper that two physical quantities which are described by two non-commuting operators (say, position and momentum) can have simultaneous reality which was a contradictory statement to the quantum theory.

However, even in the presence of such discrepancies, several predictions of quantum mechanical theory have been proved experimentally. Hence, EPR suggested the existence of certain hidden variables along with the wave function description of a physical system, so that, the theory of quantum mechanics can be considered complete. To discuss the viewpoint of EPR let us now introduce two important notions *locality* and *realism* to classify the classical world, which can be spelled as:

Locality: If two systems are interacted with each other and then separated with each other, then a measurement made on any one of them will not disturb the other system, instantaneously.

Realism: Each and every element of reality has a predefined value, i.e., each observable has its definite value irrespective of the fact that the measurement is made or not. Measurement processes just reveal those values to us.

EPR formulated their argument in terms of position and momentum observables, while D. Bohm formulated the same idea in terms of spin [100] which was conceptually simpler. He

assumed a pair of spin-$1/2$ particles in a spin singlet state such as

$$|\psi\rangle = \frac{1}{2}(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle) \tag{2.1}$$

where $|\uparrow\rangle$ (up spin) and $|\downarrow\rangle$ (down spin) states form the orthonormal basis for spin measurement. If the spin of both the particles is measured along a specific direction (say z-axis), then according to the quantum theory, results will be perfectly anti-correlated, i.e., exactly opposite to each other. If measurements are made simultaneously on two spatially-separated particles, then locality-assumption requires that any disturbance triggered by the measurement on one side cannot influence the result of the measurement on the other side. Therefore, in the presence of locality, the only way to ensure the perfect anti-correlation between the results on the two sides is to have each particle with a pre-existing determinate value. This situation is valid for a measurement made in any direction, i.e., the results of the measurements made on two correlated systems should be perfectly anti-correlated along any specific direction.

Using this result, one can immediately write for measurements made only on a single system that:

$$P(J_A^1 = J_B^1) + P(J_B^1 = J_C^1) + P(J_C^1 = J_A^1) \geq 1$$

where $P(J_A^1 = J_B^1)$ is the probability of measurement outcome in A direction being equal to the outcome in B direction for system 1. If the measurements made on the other system (correlated with the previous one) are represented by notations as J_A^2, J_B^2 and so on, then to establish perfect anti-correlation $J_A^1 = -J_A^2$, which implies that $P(J_A^1 = J_B^1) = P(J_A^1 \neq J_B^1)$, one can write

$$P(J_A^1 = J_B^2) + P(J_B^1 = J_C^2) + P(J_C^1 = J_A^2) \geq 1. \tag{2.2}$$

According to quantum theory, when spin measurements are performed on the pair of particles in the singlet state, along different axes, the probability that the two results will be opposite (one "up" and one "down") is given by $(1 + \cos(\theta))/2$, $\theta \in [0, \pi]$ where θ is the angle between two chosen axes. Now, if the measurements are made in three particular directions lying in a single plane at the angle $2\pi/3$ with each other, then $(1 + \cos(\theta))/2 = 1/4$. Hence, the inequality (2.2) is violated by quantum mechanical predictions which indicates that quantum mechanics can not be explained by local-realist theories. This result is known as the so called *Bell's theorem*.

John Bell, in 1964, used the correlation parameter $C(A, B) = E(J_A^1 J_B^2)$, defined as the expected value of the product $J_A^1 J_B^2$ of measurement outcomes on system 1 and 2, in the direction A and B, such as

$$C(A, B) = E(J_A^1 J_B^2) = P(J_A^1 J_B^2 = 1) - P(J_A^1 J_B^2 = -1) = 1 - 2P(J_A^1 J_B^2 \neq 1),$$

to construct an inequality based on the assumptions of locality & realism like the inequality (2.2) and can be written as

$$|C(A, B) - C(A, C)| \leq 1 + C(B, C). \tag{2.3}$$

If this inequality is satisfied by quantum mechanical system having correlated measurement outcomes, it means that the system shows local-realistic behaviour. However, it has been seen in experiments, so far, that the inequality (2.3) is always violated by quantum mechanical systems.

One can think of writing the joint probability of measurements made on two correlated systems as product of probabilities (independent of each other) of obtaining certain outcome for each system, i.e., $p_{A,B}(a, b|\lambda) = p_A(a|\lambda).p_B(b|\lambda)$, which represents that when two systems are separated with each other after having the interaction, any additional randomness that might affect system 1 must be independent of any additional randomness that might affect system 2 (i.e.,

condition of locality). In this case, the dependence of correlation between the outcomes on two sides should come from certain extra variable λ. More precisely, locality requires that some set of data λ made available to both systems by a common source must fully account for the dependence between two outcomes. Consequently, for a system of two correlated subsystems (particles) the probability of a coincidence between separated measurements of particles with correlated orientation properties should be written as:

$$\begin{aligned} P(a,b) &= \int d\lambda.\rho(\lambda).p_{A,B}(a,b|\lambda) \\ &= \int d\lambda.\rho(\lambda).p_A(a|\lambda).p_B(b|\lambda) \end{aligned} \tag{2.4}$$

representing the factorizability condition, where $p_A(a|\lambda)$ is the probability of detection of particle A with hidden variable λ by detector A, set in direction a, and similarly $p_B(b|\lambda)$ is the probability at detector B, set in direction b, for particle B, sharing the same value of λ. The source is assumed to produce particles A & B in the state λ with probability $\rho(\lambda)$. The probability in Eq. (2.4) represents both the locality and realism assumptions together in a mathematical formulation. The parameter λ can be considered as a hidden variable. The theory that includes hidden-variables with probabilistic or wave function description of physical reality to incorporate the requirements of locality and realism is called *local hidden-variable theory*.

Till 1990, these correlations (specifically *quantum correlations*) were regarded as physical curiosity. However after some time, it was observed that the knowledge of the nature of correlations shared by two or more subsystems of a given system can be used to perform various quantum information processing and computational tasks. To understand this, let us consider a simple example of bipartite system consisting of two subsystems A and B in the states $|\psi_A\rangle$ and $|\psi_B\rangle$ with their associated Hilbert spaces H_A and H_B, respectively. Then the total system would acquire the Hilbert space $H_A \otimes H_B$. Quantum correlations, then, can be divided into different categories, some of them are given below:

- Entanglement: If the state $|\psi_{AB}\rangle$ of the total system can be written as $|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$, then the two subsystems are independent from each other, i.e., the states of individual systems are separable. Otherwise, the state $|\psi_{AB}\rangle$ is called entangled. Quantum mechanics also allows the superposition states as given below:

  $$|\phi\rangle = \frac{1}{N}(|\phi_1\rangle \otimes b\,|\phi_2\rangle + |\phi_2\rangle \otimes b\,|\phi_1\rangle)$$

  with N as normalization constant. It can be seen that this state is non-separable, i.e., entangled. Hence, entanglement assures the quantumness of the given state.

  The usefulness of a quantum state for quantum information tasks is usually quantified by the amount of entanglement contained in the state. To transmit some information from one point (sender) to the other distinct point (receiver), both of them need to share entangled singlets. On this behalf, one of the most popular quantifiers, the distillable entanglement [101] has been proposed, which is defined as the maximal number of singlets that can be obtained per copy of a given mixed state via local operations and classical communication, if the number of copies goes to infinity. In other words, entanglement measures quantify how much a quantum state ρ fails to be separable. However, it is not always feasible to evaluate distillable entanglement for every system. Thus, its exact expressions are only known in a few special cases. For this reason, other quantifiers, known as entanglement measures, have been proposed. In this thesis, the entanglement measures based on the von-Neumann entropy (which is also a measure of information contained in a system) have been discussed.

  An entanglement measure fulfills the following properties:

- it does not increase under local operations and classical communication,
- it vanishes in case of separable states.

For a pure state $|\psi_{AB}\rangle$ the entanglement is usually quantified by the von-Neumann entropy of the reduced density matrix $\rho_j = Tr_{\text{all but not subsystem j}} |\psi_{AB}\rangle \langle\psi_{AB}|$ such as,

$$\mathcal{S} = -\sum_j Tr(\rho_j \log_2 \rho_j) \equiv -\sum_j \lambda_j \log_2 \lambda_j \tag{2.5}$$

where λ_j are eigenvalues of ρ_j. The measure given in Eq. (2.5) gives nonzero value if the state is entangled over at least one bipartite section. In this sense, it can be considered as a measure of *absolute entanglement*. $\mathcal{S} = 0$ for separable states and $\log_2 d$ for completely entangled state where d is dimension of the given system. A measure of *genuine entanglement* can also be constructed. For example, for a three party system, it can be given by the cube of geometric mean of von-Neumann entropies H for every bipartition, such as

$$\mathcal{G} = H(1|23)H(2|13)H(3|12)$$

The nonzero value of this measure implies that all the subsystems or parties are entangled with each other.

- Quantum discord: Entanglement is not necessary for a system to exhibit nonclassical correlations. In other words, it is not necessary that every separable state is classically correlated, although every classically correlated state is separable. If the state of the total system is given by $\rho_{tot} = \sum_i p_i |a_i\rangle \langle a_i| \otimes |b_i\rangle \langle b_i|$, where $|a_i\rangle$ and $|b_i\rangle$ are not orthogonal in there respective Hilbert spaces with $\sum_i p_i = 1$ and $p_i \geq 0$, then also the system can have quantum correlations in the sense of nonzero *quantum discord*. The concept of quantumness as measured by quantum discord can be essentially explained as the impossibility of measuring a quantum state without disturbing it [4, 102]. For a pure state, quantum discord can be put in one-to-one correspondence with entanglement [103], but unlike entanglement it can be nonzero for separable mixed states. Therefore, it is not studied in this thesis for neutrinos as they are produced as a pure state in weak interactions (although lepton number violating charged current interaction can cause the production of neutrinos in a mixed state, but the coupling strength of these interactions obtained from various experimental data are very small and hence are neglected in this work).

- Nonlocality: Nonlocality is another form of quantum correlation which is stronger than entanglement. This can be understood in the sense that quantum correlations shared between the subsystems of an entangled state are not necessarily nonlocal in nature. On the other hand, if a state is showing nonlocality feature then it has to be entangled. Without entanglement there is no meaning of talking about nonlocality. Thus, the existence of nonlocality gives a stronger evidence for nonclassical or quantum behaviour of the system. Bell-CHSH inequality is one of the nonlocality witnesses that holds good for a two level system. The CHSH inequality can be used in the proof of Bell's theorem, which states that certain consequences of entanglement in quantum mechanics cannot be reproduced by local hidden variable theories. Here, CHSH stands for John Clauser, Michael Horne, Abner Shimony, and Richard Holt, who described it in their paper published in 1969 [104]. The general form of Bell-CHSH inequality is given as

$$E(a,b) - E(a,b') + E(a',b) + E(a',b') \leq 2$$

where $E(a,b)$ is the average of the product of the measurement outcomes of A and B respectively in specific directions a and b and given as

$$E(a,b) = \int d\lambda \rho(\lambda) A(a,\lambda) B(b,\lambda)$$

with the average outcomes $A(a, \lambda)$ and $B(b, \lambda)$ of the settings of the detector A in a direction and the detector B in the b direction. Here, detectors A and B are supposed to perform measurements on the two entangled subsystems A and B. a, a', b and b' are alternative settings of these detectors. The CHSH inequality can also be written in a convenient way such as

$$\left\langle AB - AB' + A'B + A'B' \right\rangle \leq 2$$

There are some other Bell-type inequalities available for higher dimensional systems such as *Mermin* (M_1, $M_2 \leq 2$) [105] and *Svetlichny inequalities* ($\sigma \leq 4$) [106], where

$$\begin{aligned} M_1 &\equiv \left\langle ABC' + AB'C + A'BC - A'B'C' \right\rangle \leq 2, \\ M_2 &\equiv \left\langle ABC - A'B'C - A'BC' - AB'C' \right\rangle \leq 2, \end{aligned} \tag{2.6}$$

and

$$\sigma \equiv M_1 + M_2 \leq 4. \tag{2.7}$$

For the systems having dimensions greater than 2, it becomes more interesting to know how the correlations are distributed among all the subsystems. For example, in case of a three-party-system it may be possible that either (i) every subsystem is locally correlated with each other, (ii) or two of them are nonlocally correlated with each other and having local correlation with the third one, (iii) or all the subsystems are correlated with each other nonlocally. In the first, case both Mermin and Svetlichny inequalities will be satisfied by the total system, while in the second case, Mermin inequalities will be violated and svetlichny inequality will be satisfied. For the third case, both of these inequalities will be violated by the system. In this sense the Mermin parameters M_1, M_2 can be considered as an absolute measure of tripartite nonlocality. On the other hand σ defining the Svetlichny parameter can stand as a genuine tripartite nonlocality measure. The violation of these inequalities mentioned here implies nonlocality in a manner that the quantum correlations cannot be modelled classically with particles assuming definite, localized properties.

- Steering: An intermediate feature between entanglement and nonlocality is known as steering. Unlike nonlocality, the steering measure implies the asymmetric nonlocal correlation between the subsystems of a given system. This means that one can manipulate or steer one subsystem by performing the local operation on the other but this will not be true for the reverse case. While the entanglement and nonlocality can be considered symmetric nonclassicality measures [107, 108].

The hierarchy of the strongness of these measures to imply the nonclassical behaviour of the system can be understood in Fig. 2.1.

Temporal correlations: Various measures discussed so far represent the spatial nonclassical features present in the system. A temporal counterpart of nonlocality is known as *Leggett-Garg inequality* [5] which is based on the concept of *macrorealism* and *noninvasive measurements* (NIM). Here, macrorealism implies that if a system consisting of two macroscopically distinct states corresponding to a measurement $O(t)$, then the system will definitely exist in one of these states irrespective of any measurement performed on it. (NIM) signify that a measurement can be performed without disturbing the future dynamics of the system.

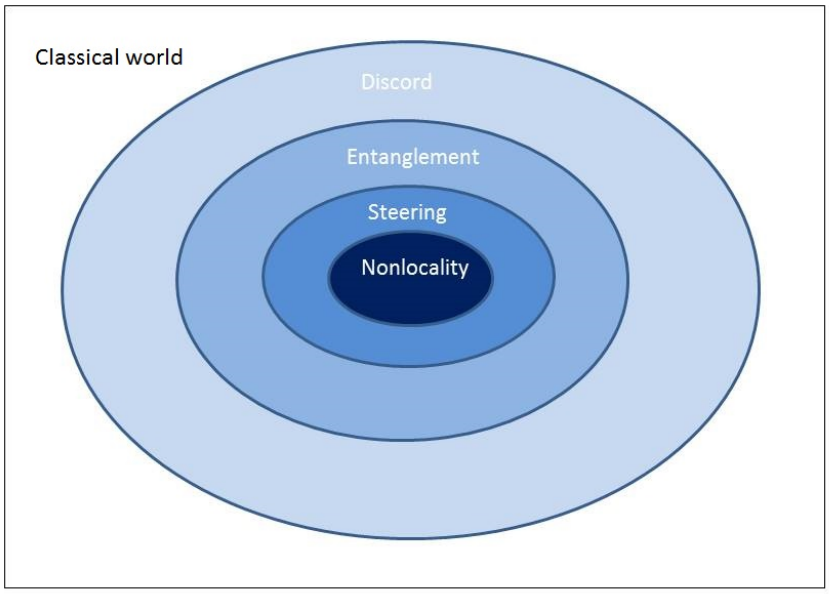

Figure 2.1: Hierarchy of the strength of various nonclassicality measures has been described here. It can be seen that nonlocality is the subset of all the classes defined here which means a system showing nonlocality will definitely carry the quantum correlations defined by the steering, entanglement and quantum discord. Hence, nonlocality is the strongest measure of nonclassical features so far. In this figure, the darker is the blue color, the stronger is the measure.

2.2 Quantum coherence

The most essential feature in the theory of quantum mechanics is the superposition principle and the quantum mechanical phenomena such as interference appears due to the existence of *quantum coherence*. Basically, quantum coherence has the potential to establish a boundary between the classical and the quantum world. Quantum coherence is also a necessary condition for both entanglement and other types of quantum correlations. In *quantum resource theories*, quantum coherence is a key element and a primary facilitator for design and implementation of quantum technologies. The quantum physical phenomena such as entanglement and the nonlocal quantum correlations were originally pioneered to meticulously demean the opponents of quantum mechanics, which are now thought to be reassessed to elevate them as resources to achieve tasks that are not possible within the domain of classical physics. In this line, the detection, quantification and optimization of these quantum effects should be carried out vigorously which is the basic idea of the development of quantum resource theories.

Quantum resource theories mainly address three fundamental issues such as, (i) characterization, (ii) quantification and (iii) the manipulation of quantum states and the imposed constraints on those states. An example of these constraints can be the limitation of local operations and classical communication (LOCC). In the context of quantum information theory, the quantification of coherence can be done based on the characterization of the set of incoherent states ($\mathcal{I}$) and incoherent operations ($\mathcal{O}^{\mathcal{I}}$). In a given reference basis $\{|i\rangle\}$, states defined as $\rho_{\mathcal{I}} = \sum_i d_i \, |i\rangle \langle i|$ where $d_i \geq 0$ and $\sum_i d_i = 1$, form a set of incoherent states. Incoherent operations are specified in such a manner that they map the set of incoherent states onto itself, i.e., $\mathcal{O}^{\mathcal{I}}(\mathcal{I}) \in \mathcal{I}$. In such a set of incoherent operations ($\mathcal{O}^{\mathcal{I}}$) and incoherent states ($\mathcal{I}$), the l_1-norm (sum of the absolute values of

off-diagonal elements of the density matrix $\rho = |\psi\rangle\langle\psi|$) [35, 109]

$$\chi = \sum_{i \neq j} |\rho_{ij}| \tag{2.8}$$

represents a reliable measure or quantifier of coherence since it acquires all the basic properties of a coherence-measure such as, (i) non-negativity, i.e. $\chi(\rho) = 0$ iff $\rho \in \mathcal{I}$, (ii) monotonicity under incoherent operations, in other words, $\chi(\rho)$ is nonicreasing under the incoherent operations, i.e., $\chi(\mathcal{O}^{\mathcal{I}}[\rho]) \leq \chi(\rho)$ and (iii) convexity, i.e., $\chi(\sum_k p_k \rho_k) \leq \sum_k p_k \chi(\rho_k)$, where $\rho_k = Q_k \rho Q_k^\dagger / p_k$ (Q_k is the Kraus operator) and $p_k = Tr(Q_k \rho Q_k^\dagger)$. The value of this measure for a d-dimensional maximally coherent state defined by $|\psi_d\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle$ becomes $d-1$, placing the upper bound (or maximal value) on this measure. While χ is zero for a completely incoherent state.

Some other well known measures of quantum coherence, satisfying the above mentioned properties required for a quantum-measure, are those based on relative entropy [35, 38] and skew-information [39]. Further, it has been recently shown that measures of entanglement can be put to use to understand quantum coherence [40].

2.3 Geometric Phase

As the theory of quantum mechanics evolved, it came out with several other interesting phenomena leading to our knowledge about nature up to the next step. Some of those features have been discussed in previous sections such as entanglement, nonlocality and quantum coherence. In this section another intriguing feature, the geometric phase (GP) is discussed that provides the information about the path taken by the system during its time evolution. GP has a rich and interesting history. It was introduced by M. Berry [110] in 1984, for the case of cyclic and adiabatic evolution of a quantum system under the action of a time-dependent Hamiltonian and he called this the Berry phase. However, it was later pointed out by Nityananda and Ramaseshan [111] that Pancharatnam, in 1956, has already provided a generalized version of the Berry phase for polarized lights. Later on, This GP was analyzed for non-adiabatic [112] and non-cyclic cases [113] also.

2.3.1 Berry phase

Berry's phase was based on the *adiabatic theorem* which states that if the Hamiltonian of the system changes gradually from H^i to final form H^f (i.e., the time scale of the system's evolution is much shorter than the time scale of changing Hamiltonian) then the system started in the n^{th} eigenstate of H^i will be carried out under the Schrödinger equation into the n^{th} eigenstate of H^f picking up only a phase factor. This can be understood in the following way:

A state vector associated with a Hilbert space $\mathcal{H}$ contains the information of a system and the dynamics of the system's evolution is governed by the Schrodinger equation. For a static system, i.e., for a time-independent Hamiltonian, the time evolution is given by

$$H\psi_n = E_n \psi_n$$

The energy eigenstate ψ_n of the system remains unchanged after this evolution. This is an example of the ideal case. In general, a system is not completely isolated with its surroundings and hence, the Hamiltonian should be time-dependent. However, the condition of adiabaticity provides us the space to approximate the time dependent evolution as a static case. Considering the evolution of a quantum system under the action of a time-dependent Hamiltonian H(t) (that happens when the system interacts with the environment) and a set of parameters $(R_1, R_2, \dots)$ representing the configuration of the environment, the evolution of the system can be given by Schrodinger equation,

or more generally, by the Liouville-von Neumann equation

$$i\frac{d\rho(t)}{dt} = [H(R(t)), \rho(t)],$$

where $\rho = |\psi\rangle\langle\psi|$ is the density matrix operator describing a pure state. An environmental process can be described as a curve obtained by the vector R in parameter space which corresponds to a curve described by $|\psi(t)\rangle$ in its associated Hilbert space $\mathcal{H}$ or to the curve defined by $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ in the associated projection space $\mathcal{P}(\mathcal{H})$. Then, we assume that for all R there is an orthonormal and non degenerate eigenbasis $|n; R\rangle$ such as

$$H(R(t))\,|n; R(t)\rangle = E_n(R(t))\,|n; R(t)\rangle\,. \tag{2.9}$$

Differentiating Eq. (2.9) we have

$$\dot{H}\,|n\rangle + H\,|\dot{n}\rangle = \dot{E}_n\,|n\rangle + E_n\,|\dot{n}\rangle$$

and taking its inner product with $\langle m; R(t)|$ we are left with

$$\langle m|\dot{n}\rangle = \frac{\langle m|\dot{H}|n\rangle}{|E_n - E_m|}.$$

Then according to the *adiabatic theorem*

$$\langle m|\dot{H}|n\rangle \ll \frac{|E_n - E_m|}{\Delta T_{mn}}$$

Here ΔT_{mn} is the characteristic transition time of the system between states $|m\rangle$ and $|n\rangle$. Then the adiabatic limit can be spelled out as $\langle m; R|\dot{H}|n; R\rangle \approx 0$ in the limit of $\Delta T_{mn} \gg 1$. The final state of the system can be expanded into the energy eigenstate basis

$$|\Psi(t)\rangle = \sum_n c_n(t) e^{-\frac{i}{\hbar}\int_0^t E_n(\tau)d\tau}\,|n; R(t)\rangle \tag{2.10}$$

Substituting Eq. (2.10) into the Schrodinger eq. we get

$$\dot{c}_n(t) = -c_n(0)\langle n|\dot{n}\rangle - \sum_{n\neq m} c_n \frac{\langle m|\dot{H}|n\rangle}{E_n - E_m} e^{-\frac{i}{\hbar}\int_0^t (E_n(\tau) - E_m(\tau))d\tau}$$

Under the adiabatic condition, the second terms on the right hand side drops out and the solution of the above eq. reads,

$$c_n(t) = c_n(0) Exp[-\int_0^t \langle n(R(\tau))|\frac{d}{dt}|n(R(\tau))\rangle d\tau] = c_n(0) e^{i\gamma_n(t)}.$$

If the system starts out in the n^{th} eigenstate, i.e., $c_n(0) = 1$ and $c_n(0) = 0$ for $m \neq n$, then Eq. (2.10) becomes

$$|\Psi(t)\rangle = e^{i\phi_{total}}\,|n; R\rangle \equiv e^{i\theta_n(t)} e^{i\gamma_n(t)}\,|n; R\rangle$$

where $\theta_n(t)$ and $\gamma_n(t)$ are the dynamical and geometrical phases and given by

$$\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')dt',$$

$$\gamma_n(t) \equiv i\int_0^t \langle n; R(t')|\frac{\partial}{\partial t}|n; R(t')\rangle dt' \equiv i\int_{R_i}^{R_f} \langle n; R|\Delta_R|n; R\rangle dR.$$

Here we have used the relation $\frac{\partial|n;R\rangle}{\partial t} = \nabla_R |n;R\rangle \frac{dR}{dt}$ with ∇_R being the gradient in the parameter space $\mathbf{R} \equiv (R_1, R_2, ...)$. The cyclic nature of the environmental process is given in the sense that $R(T) = R(0)$, $E_n(R(T)) = E_n(R(0))$ and $|n;R(T)\rangle \langle n;R(T)| = |n;R(0)\rangle \langle n;R(0)|$. Hence, if the Hamiltonian returns to its original form after time T, then the net geometric phase can be expressed as

$$\boxed{\gamma_n(t) \equiv i \oint \langle n;R|\nabla_R|n;R\rangle.dR = \oint A_n(R)}.$$

We can see that in contrast with the dynamical phase, an extra phase γ_n appears in the system's evolution. Notice that γ_n is determined by the path taken during the adiabatic evolution in the parameter space, and it is independent of the rate at which the system is evolving. This is why the phase γ_n is called the geometric phase due to its geometry origin. The geometric phase given in the box above is called Berry phase under the cyclic and adiabatic condition. The quantity $A_n(R) = i\langle n;R|\nabla_R|n;R\rangle$ is called Berry's connection. We should also notice that the Hamiltonian is needed to have two or more parameters owing its time dependence. In case of single parameter $R(t)$, after a complete cycle $R(T) = R(0) \Rightarrow \gamma_n(T) = 0$. Another noticeable point is that the quantity $\langle n;R|\nabla_R|n;R\rangle$ is purely imaginary, hence, the eigenfunctions of the Hamiltonian must be complex eigenfunctions for a non-zero value of geometric phase. Since $Re(\langle n;R|\Delta_R|n;R\rangle) = 0$, hence $\gamma_n(t)$ is real.

Now let's look at the gauge transformation of the form

$$|n';R\rangle = e^{-i\beta(R)} |n;R\rangle \tag{2.11}$$

with $\beta(R) \rightarrow$ real. Then, the state $|n';R\rangle$ also satisfies the Schrodinger eq., i.e.,

$$H(R(t)) |n';R(t)\rangle = E_n(R(t)) |n';R(t)\rangle .$$

The quantity $A_n(R)$ transforms under the gauge transformation (2.11) as

$$\begin{aligned} A'_n &= i\langle n;R|e^{i\beta(R)}\nabla_R e^{-i\beta(R)}|n;R\rangle \\ &= A_n(R) + \nabla_R\beta(R). \end{aligned} \tag{2.12}$$

It can be seen that A_n transforms as vector potential under the gauge transformation (2.11). Now if the system evolves along the path Γ in the parameter space while going from R_i to R_f, then the transformation of γ_n can be given as

$$\begin{aligned} \gamma'_n(\Gamma) &= \int_\Gamma A'_n(R).dR \\ &= \int_\Gamma A_n(R).dR + \int_{R_i}^{R_f} \nabla_R\beta.dR \\ &= \gamma_n(\Gamma) + \int_{R_i}^{R_f} \nabla_R\beta.dR \end{aligned} \tag{2.13}$$

or

$$\gamma'_n(\Gamma) = \gamma_n(\Gamma) + \beta(R_f) - \beta(R_i) \tag{2.14}$$

From Eq. (2.14) it is clear that γ_n is not gauge invariant except at the condition $R_f = R_i$, since, then $\beta(R_i) = \beta(R_f)$, i.e., geometric phase is invariant only for a closed path (when the system completes one cycle) in the parameter space. After n cycles, $\gamma'_n(\Gamma) = \gamma_n(\Gamma) + 2n\pi$.

Remarks:

We have seen that Berry's work was based on some assumptions, such as

- the time evolution of given system is governed by the Schrodinger eq. with hermitian Hamiltonian H, i.e., the evolution is unitary,
- evolution should be adiabatic, i.e., H should vary very slowly with time,
- evolution should be cyclic, (i.e., Hamiltonian should vary cyclically or $H(T) = H(0)$).

The connection of this work to the earlier work of Pancharatnam [114] related to the interference of polarized light was made in [111].

2.3.2 Generalization of Berry phase

Aharonov and Anandan (AA) phase: So far we have seen that Berry's phase was based on the adiabatic theorem and hence, it was assumed that system should be initially in one of the eigenstates of the Hamiltonian. Aharonov and Anandan in 1986 [112], showed that the geometric phase can appear for cyclic evolution of any arbitrary quantum state vector $|\psi(t)\rangle$ and the evolution is allowed to be non-adiabatic. Also, from cyclic evolution it is meant that $|\psi(T)\rangle = |\psi(0)\rangle$ (not the cyclicity of $H(t)$).

Let us first consider a projective Hilbert space $\mathcal{P}$ that consists of the equivalence classes of all state vectors (also called ray space) of the Hilbert space $\mathcal{H}$, i.e., the set of state vectors connected with each other via a complex number such as $|\psi'\rangle = c\,|\psi\rangle$, $c \in \mathbb{C}$. Then, the projection map Π form Hilbert space $\mathcal{H}$ into the projective space $\mathcal{P}$ is defined by $\Pi : \mathcal{H} \to \mathcal{P}$, such as

$$\Pi(|\psi\rangle) = \{|\psi'\rangle : |\psi'\rangle = c\,|\psi\rangle\,, c \in \mathbb{C}\} \tag{2.15}$$

AA showed that the geometric phase depends neither on the phase factor relating the initial and final state vectors nor on the Hamiltonian H. Geometric phase associated with the cyclic evolution of the state vector is universal in the sense that it remains unchanged for the infinite number of possible motions along the curves in the Hilbert space $\mathcal{H}$ that project onto a single closed curve in the projective Hilbert space $\mathcal{P}$ of rays and the Hamiltonians through which the states evolve along those curves. Let us now consider a normalized state $|\psi(t)\rangle \in \mathcal{H}$ such that $|\psi(\tau)\rangle = e^{i\phi}\,|\psi(0)\rangle$ and the Schrodinger eq. is given by

$$H(t)\,|\psi(t)\rangle = i\hbar\frac{d}{dt}\,|\psi(t)\rangle \tag{2.16}$$

and the projection map is defined in Eq. (2.15). Then during the evolution $|\psi(t)\rangle$ defines a curve $C : [0, \tau] \to \mathcal{H}$ with $\hat{C} \equiv \Pi(C)$ being a closed curve in $\mathcal{P}$. Now, defining the state

$$|\tilde{\psi}(t)\rangle = e^{-if(t)}\,|\psi(t)\rangle\,, \tag{2.17}$$

such that $f(\tau) - f(0) = \phi$, it is easy to get that $|\tilde{\psi}(t)\rangle = |\tilde{\psi}(0)\rangle$. Inserting Eq. (2.17) in (2.16) we have

$$\hbar\frac{d}{dt}f(t) = i\langle\tilde{\psi}(t)|\frac{\partial}{\partial t}|\tilde{\psi}(t)\rangle - \langle\tilde{\psi}(t)|H|\tilde{\psi}(t)\rangle$$

Then using the relation

$$\int_0^\tau \frac{d}{dt}f(t)dt = \phi = \theta + \beta$$

one can figure out that

$$\theta \equiv -\frac{1}{\hbar}\int_0^\tau \langle\tilde{\psi}(t)|H|\tilde{\psi}(t)\rangle dt$$

is the dynamical phase and

$$\beta = \int_0^\tau \langle\tilde{\psi}(t)|i\frac{d}{dt}|\tilde{\psi}(t)\rangle dt \tag{2.18}$$

is the geometric phase. Therefore, removing the dynamical part from the total phase ϕ one can obtain the geometric phase such as

$$\beta \equiv \phi + \frac{1}{\hbar}\int_0^\tau \langle\tilde{\psi}(t)|H|\tilde{\psi}(t)\rangle dt \tag{2.19}$$

Hence, it is clear that choosing an appropriate $f(t)$ the $|\tilde{\psi}(t)\rangle$ can be chosen for every curve C in Hilbert space $\mathcal{H}$ which projects onto a single closed curve $\Pi(C) \equiv \hat{C}$ in the projective Hilbert space or the ray-space $\mathcal{P}$. From Eq. (2.18) it is clear that β is independent of ϕ and Hamiltonian H. Actually, for a given curve C in $\mathcal{H}$, the Hamiltonian $H(t)$ can be chosen such that the second term on right hand side of Eq. (2.19) vanish and the total phase ϕ will be completely equal to β, i,e. the geometric part. It can be said that β is the geometric phase associated with a closed curve in the projective Hilbert space $\mathcal{P}$ and does not depend on the parameter space. Also, unlike the limiting case considered by Berry, $|\psi(t)\rangle$ need not be an eigenstate of $H(t)$.

Noncyclic phase by Samuel and Bhandari: Next step was taken by J. Samuel and R. Bhandari [113], in 1988, to show that the cyclicity condition is also not necessary to define a nonzero geometric phase. They coined the term of geodesic to prove their statement. They stated that if a system starts in a state $\psi(0)$ and after time t, alog the curve $\mathcal{C}$ it reaches $\psi(t)$, then having a unique geodesic connecting the state $\psi(t)$ back to the state $\psi(0)$, one will obtain a nonzero geometric phase. Here, geodesic is defined as a curve in ray space $\mathcal{R}$ connecting the two points ρ_1 and ρ_2 if the length functional corresponding to this curve is minimum. The length functional is defined as

$$L[C] = \int_{S_1}^{S_2} dS\{(\dot{\psi}(S),\dot{\psi}(S)) - (\psi(S),\dot{\psi}(S))(\dot{\psi}(S),\psi(S))\}^{1/2},$$

where $(\dot{\psi}(S),\dot{\psi}(S))$ represents the inner product of $\dot{\psi}(S)$ with itself and $\dot{\psi}(S) = \frac{d\psi}{dS}$.