The Adiabatic theorem and "Berry's Phase"*

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A. Statement of the problem.

Suppose our Hamiltonian, $H(s)$, depends on a parameter s, and furthermore let us assume that it has discrete eigenstates, indexed by m, such that,

$$H(s)\,|m, s\rangle = E_m(s)\,|m, s\rangle. \tag{1}$$

Wie shall assume that over some range of s, the eigenstates are non-degenerate, so that we can unambiguously order them in terms of their energies, $E_m > E_k$ for $m > k$. Furthermore, let us also suppose that there exists a minimum value of the energy gap, Δ, between some particular state n and all other states, over the given range of s.

Let the parameter, s, now vary slowly in time during the interval, $-\tau < t < \tau$, with τ large, such that

$$s(t) = \begin{cases} s_i \ \text{ at } \ t = -\tau, \\ \\ s_f \ \text{ at } \ t = +\tau. \end{cases} \tag{2}$$

To make this precise, we can write $s = f(t/\tau)$, where f is an arbitrary smooth function such that $f(-1) = s_i$ and $f(1) = s_f$, and we can take the limit where τ becomes large.

We want to study a state, $|\psi(t)\rangle$ that satisfies the Schrödinger equation,

$$i\hbar\partial_\tau\,|\psi(t)\rangle = H(s)\,|\psi(t)\rangle, \tag{3}$$

with the initial condition, $|\psi(-\tau)\rangle = |n, s_i\rangle$.; i.e.,it starts inan eigenstate of $H(s_i)$. According to the *adiabatic theorem*, in the limit of $\tau \to \infty$, $|\psi(\tau)\rangle$ will be in the corresponding eigenstate $|n, s_f\rangle$, except for some small corrections that vanish under the same limit, i.e.

$$|\psi(t = \tau)\rangle = e^{i\phi}|n, s_f\rangle + O\Big(\frac{1}{\tau}\Big), \tag{4}$$

where the correction can actually be $\ll 1/\tau$. We shall prove the above statement and will also investigate the nature of the phase, ϕ.

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B. Proof

We start with the claim, in the limit of large τ, that,

$$\phi = \phi_{\rm dyn} + \gamma_n, \tag{5}$$

$$\phi_{\rm dyn} = -\frac{1}{\hbar}\int_{-\tau}^{\tau} E_n(s)\, dt, \tag{6}$$

$$\gamma_n = i\int_{-\tau}^{\tau} \langle n, s|\frac{d}{dt}|n, s\rangle\, dt. \tag{7}$$

In the above equations, $\phi_{\rm dyn}$ is just the usual phase that comes from the time evolution of the state, $|\psi(t)\rangle$, whereas γ_n is an additional term, which is commonly referred to as *Berry* phase. (See, however, the historical remarks at the end of these notes.) The above relations can be re-written as,

$$\phi_{\rm dyn} = -\frac{1}{\hbar}\int_{s_i}^{s_f} \frac{E_n(s)}{ds/dt}\, ds \propto \tau, \tag{8}$$

$$\gamma_n = i\int_{s_i}^{s_f} \langle n, s|\frac{d}{ds}|n, s\rangle\, ds, \quad \text{independent of } \tau. \tag{9}$$

The Berry phase, γ_n, is also independent of the shape of the function $f(s)$ at intermediate times.

It is straightforward to see that γ_n is purely real. This follows immediately from the normalization condition, $\langle n, s|n, s\rangle = 1$, as follows,

$$\frac{d}{ds}\langle n, s|n, s\rangle = \langle n, s|\frac{\partial}{\partial s}|n, s\rangle + \left(\langle n, s|\frac{\partial}{\partial s}|n, s\rangle\right)^* = 0. \tag{10}$$

Let us now prove the statement of the adiabatic theorem. For the sake of convenience, we shall set $\hbar = 1$. To start, we note that the value of ϕ is in some sense arbitrary. In order to really make sense of the phase, we must first specify the phases of all the eigenstates, $|n, s\rangle$. In particular, different choices will lead to different answers for ϕ.

Suppose we have made a choice such that $|n, s\rangle$ varies continuously with s and the phase is *single valued*. Then we can expand $|\psi(t)\rangle = \sum_m c_m(t)|m, s(t)\rangle$ with $c_m(t) = \langle m, s(t)|\psi(t)\rangle$. Then let us define the unitary matrix,

$$U_{mm'}(s) = \langle m, s|m', s_i\rangle\Big|_{s=s(t)}. \tag{11}$$

Then, we claim that,

$$i\frac{\partial}{\partial t}c_m(t) = E_m(s)c_m(t) + \frac{1}{\tau}\sum_{m'} V_{mm'}c_{m'}(t), \text{ where} \tag{12}$$

$$\frac{1}{\tau}V \equiv i\Big(\frac{\partial U}{\partial t}\Big)U^{-1} = i\frac{\partial s}{\partial t}\Big(\frac{\partial U}{\partial s}\Big)U^{-1}, \tag{13}$$

which is manifestly of order $1/\tau$.

We want to solve the above equations for $c_m(t)$ with the initial condition, $c_m(-\tau) = \delta_{mn}$. Then at least for short times, we know that c_m is small for $m \neq n$ and $|c_n| \approx 1$. The equation of motion for c_m is given by,

$$i\frac{\partial}{\partial t}c_n = \left[\frac{V_{nn}}{\tau} + E_n\right]c_n + \frac{1}{\tau}\sum_{m\neq n} V_{nm}c_m. \tag{14}$$

If we ignore the off diagonal terms for now, then we can solve for c_n as,

$$c_n(t) \approx e^{-iu_n(t)}e^{-i\int_{-\tau}^{t} V_{nn}dt'/\tau}, \tag{15}$$

where we have defined the quantity,

$$u_m(t) = \int_{-\tau}^{t} E_m(s(t'))dt'\Big[= O(\tau)\Big]. \tag{16}$$

Note that since U is unitary, $U^{-1} = U^\dagger \Rightarrow UU^\dagger = 1$, so that,

$$\frac{\partial U}{\partial s}U^\dagger + U\frac{\partial U^\dagger}{\partial s} = 0. \tag{17}$$

Therefore, the diagonal elements of $\frac{\partial U}{\partial s}U^\dagger$ are purely imaginary and V_{nn} is purely real. Furthermore, from the definition of V, it is straightforward to show that

$$-iV_{nn}/\tau = -\langle n, s|\frac{d}{ds}|n, s\rangle. \tag{18}$$

Therefore the second factor on the right hand side of (15) is just the Berry phase factor, $e^{i\gamma_n}$, while the first factor is clearly the dynamic phase factor.

In order to examine the effect of the term we have neglected in (14), we first calculate c_m for $m \neq n$:

$$c_m(t) \approx -ie^{-iu_m(t)}\int_{-\tau}^{t}\frac{dt'}{\tau}V_{mn}(t')e^{iu_m(t')}c_n(t'). \tag{19}$$

Since $c_n(t')$ itself varies as $e^{-iu_m(t')}$, we see that $|u_m(t') - u_n(t')|$ is $\sim t\Delta$, because $|E_n - E_m| > \Delta$. Therefore, the phase-factor varies very rapidly over the range of integral when $\tau \to \infty$, leading to the integral being small, of order $1/\tau$ or smaller. (The dominant contribution generally comes from the end point region, where t' is close to t.)

Let us now return to the term we have neglected in (14) for the time derivative of c_n. This will give a contribution to c_n of the form

$$\delta c_n(t) \sim \sum_m \int_{-\tau}^{t} dt' V_{nm}(t')e^{i[u_n(t)-u_n(t')]}c_m(t'), \tag{20}$$

which will be of order $O(1/\tau^2)$, or smaller, as the integrand is again rapidly oscillating. therefore we are justified in neglecting it in the limit of $\tau \to \infty$.

C. Case of multiple parameters.

The discussion so far has been for the case when the Hamiltonian was a function of a single parameter s. What if there are several parameters, such that the Hamiltonian, $H(\mathbf{R})$ is a function of $\mathbf{R} = R_1, R_2, ..., R_N$? Once again, suppose that $\mathbf{R}(t)$ varies slowly along some path from $\mathbf{R}_i$ to $\mathbf{R}_f$ in a region S, within which he eigenstates, $|m, \mathbf{R}\rangle$ are supposed to be non-degenerate and the phases are well defined. If initially,

$$|\psi(-\tau)\rangle = |n, R_i\rangle, \tag{21}$$

then the same arguments lead to $\psi(\tau)\rangle = |n, R_f\rangle e^{i\phi}$, where,

$$\phi = \phi_{\rm dyn} + \gamma_n, \text{ where} \tag{22}$$

$$\phi_{\rm dyn} = -\int_{-\tau}^{\tau} E_n(t)\, dt, \tag{23}$$

and the Berry phase is given by,

$$\gamma_n = i\int_{-\tau}^{\tau} \langle n, \mathbf{R}|\frac{d}{dt}|n, \mathbf{R}\rangle = \int_{\mathbf{R}_i}^{\mathbf{R}_f} d\mathbf{R}\cdot\mathbf{A}(\mathbf{R}), \tag{24}$$

where the *vector-potential*, $\mathbf{A}(\mathbf{R})$, is defined as,

$$\mathbf{A}(\mathbf{R}) = i\langle n, \mathbf{R}|\frac{\partial}{\partial\mathbf{R}}|n, \mathbf{R}\rangle = -{\rm Im}\langle n, \mathbf{R}|\frac{\partial}{\partial\mathbf{R}}|n, \mathbf{R}\rangle. \tag{25}$$

$\mathbf{A}(\mathbf{R})$ as defined above is an $N-$component vector.

We have already pointed out the ambiguity associated with the definition of γ_n earlier, which is related to the choice of phases for the basis states $|n, \mathbf{R}\rangle$. Therefore, we could have made another choice, say,

$$|n, \mathbf{R}\rangle_2 = e^{i\Lambda(\mathbf{R})}|n, \mathbf{R}\rangle_1, \tag{26}$$

where Λ is an arbitrary real function of $\mathbf{R}$. It is then straightforward to see that, provided Λ is differentiable, the vector potential will be transformed to

$$\mathbf{A}^2(\mathbf{R}) = \mathbf{A}^1(\mathbf{R}) - \nabla\Lambda(\mathbf{R}). \tag{27}$$

In general, if we integrate these different vector potentials along a given path, we will find that $\gamma_n^1 \neq \gamma_n^2$. However, if the path is closed, with $|n, \mathbf{R}\rangle_1$ and $|n, \mathbf{R}\rangle_2$ single- valued and varying continuously along the entire path, then $e^{i\Lambda(\mathbf{R})}$ must be defined so that it is single valued along the path, and thus

$$\gamma_n^1 - \gamma_n^2 = \oint \nabla\Lambda\cdot d\mathbf{R} = 2\pi m, \tag{28}$$

with m = integer. Therefore, $e^{i\gamma_n}$ for a closed path is independent of the gauge choice. (Of course, we are not saying that $e^{i\gamma_n}$ for a closed path is necessarily equal to 1.)

Moreover, if we consider two different open paths, labeled α, β , between a given starting point $\mathbf{R}_i$ and a given endi point $\mathbf{R}_f$, the Berry phase $\gamma_{n\alpha}$ for path α may be different from $\gamma_{n\beta}$, for path β. However, if we combine a forward trip along path α with a backward trip along β, we obtain a single closed path, starting at R_i, passing through R_f, and returning to R_i. Therefore, we can use the results for a closed path to say the exponential of the phase-difference between the two open paths, $e^{i(\gamma_{n\alpha}-\gamma_{n\beta})}$, will not depend on the particular choice of gauge.

We next define a *Berry curvature*,

$$F_{jk}(\mathbf{R}) = \Big(\frac{\partial A_k}{\partial R_j} - \frac{\partial A_j}{\partial R_k}\Big). \tag{29}$$

It is easy to see that F_{jk} is independent of the choice of gauge, provided that the vector potential is continuous and differentiable at the point $\mathbf{R}$.

Let us now talk more about closed paths, when $\mathbf{R}_i = \mathbf{R}_f$. Once again, we have $\gamma_n = \oint \mathbf{A}(\mathbf{R}) \cdot d\mathbf{R}$. If there exists a surface S spanning the closed path which lies entirely in a region where $\mathbf{A}$ is defined and is continuous and differentiable, then via Stokes' theorem, we can express γ_n as an integral of F_{jk} over the surface. As an example, if $\mathbf{R}$ is a 3−component vector, then we can define a *magnetic-field*,

$$\mathbf{B}_j = \frac{1}{2}\varepsilon_{jkl}F_{kl}. \tag{30}$$

Then $\gamma_n = \int_S \mathbf{B} \cdot d^2\vec{S}$, which can be interpreted as a "flux through the surface" and is clearly independent of the choice of gauge. Similarly, if $\mathbf{R}$ is a 2−component vector, $B = F_{12}$ (B is now a scalar), and $\gamma_n = \int_S B\, d^2S$, again independent of the choice of gauge.

D. Application: Two-level system a time-dependent "magnetic field".

We consider a two level system with a time-dependent Hamiltonian given by,

$$H = \mathbf{b}(t) \cdot \vec{\sigma}. \tag{31}$$

In this problem, the analog of the parameter, $\mathbf{R}$, introduced earlier is the magnetic-field, $\mathbf{b}$ (with 3 parameters). Let us assume that $\mathbf{b} \neq 0$ at all times and $|\mathbf{b}| > \Delta$. The condition for a slowly varying field is given by, $|d\mathbf{b}/dt| \ll \mathbf{b}$ at all times. The energy levels of this system are given by, $E^n_{\mathbf{b}} = \pm|\mathbf{b}|$, where the states are labeled by $n = \pm 1$.

Let us assume that initially, the state is prepared in its ground state, with $n = -1$. We still need to choose the phases of basis states. The canonical choice involves writing $\mathbf{b}$ in spherical coordinates, $\mathbf{b} = (b, \theta, \varphi)$,

where θ is the angle between $\mathbf{b}$ and $\hat{z}$, and $b > 0$. At the north-pole, $\theta = 0$, we choose,

$$|+\mathbf{b}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\mathbf{b}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{32}$$

For all other directions, other than the south pole, we choose

$$|+\mathbf{b}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{pmatrix}, \quad |-\mathbf{b}\rangle = \begin{pmatrix} \sin(\theta/2)e^{-i\varphi} \\ -\cos(\theta/2) \end{pmatrix}. \tag{33}$$

The south pole is a singular point in this gauge.

Now for the "−" state, away from the south pole,

$$\langle\mathbf{b}|\partial_\theta|\mathbf{b}\rangle = 0, \tag{34}$$

$$\langle\mathbf{b}|\partial_\varphi|\mathbf{b}\rangle = -i\sin^2(\theta/2) = -i\left(\frac{1-\cos\theta}{2}\right), \tag{35}$$

$$\langle\mathbf{b}|\partial_b|\mathbf{b}\rangle = 0. \tag{36}$$

Therefore, $\mathbf{A}$ points in the azimuthal direction, perpendicular to $\mathbf{b}$. Since $|d\mathbf{b}| = b\sin\theta\, d\varphi$, we have $|\mathbf{A}| = (1-\cos\theta)/(2b\sin\theta)$. Hence ,evaluating the Berry phase along a contour of constant latitude of length $= 2\pi b\sin\theta$, we have

$$\gamma_n = \oint \mathbf{A}\cdot d\mathbf{b} = \left(\frac{1-\cos\theta}{2}\right)\frac{2\pi b\sin\theta}{b\sin\theta} = \int_0^{2\pi} d\varphi\, i\langle\mathbf{b}|\partial_\varphi|\mathbf{b}\rangle = \pi(1-\cos\theta). \tag{37}$$

By Stokes theorem, this must be the is the flux through the surface S the surface which is enclosed by C and passes through the north pole. The area of S is clearly equal to $b^2(1-\cos\theta)$. Therefore, the "Berry field", $\mathbf{B}$, must be given by,

$$\mathbf{B} = \frac{1}{2b^2}\hat{b}. \tag{38}$$

Note that for a small contour surrounding the north pole, $\gamma_n \approx 0$. On the other hand, for a small contour surrounding the south pole, $\gamma_n \approx (4\pi b^2)/(2b^2) = 2\pi$. But in both cases, $e^{i\gamma_n} \to 1$.

Of course, we could have chosen a different gauge, where the vector potential was regular at the south pole but singular at the north pole. In this case, we would have found $\gamma_n \approx 0$, and $\gamma_n \approx -2\pi$ for a small contour encircling the north pole. In order to use Stokes theorem, we then would have to let S be the surface passing through the south pole.

As remarked above, the Berry curvature at any given point is independent of the gauge choice, as long as the gauge is not singular at that point. Therefore, to define the Berry curvature at a point, we simply use any convenient gauge that is not singular at the point in question. With this convention, we se that the field

Berry field $\mathbf{B}$ is perfectly continuous at the south pole, and is given by (38), as at all other points on the sphere.

The fact that the Berry flux $\int \mathbf{B} \cdot d^2S$ through the surface of a sphere containing the origin is 2π, and not zero, signifies the presence of a singularity (or, a degeneracy point) at the origin, inside the sphere. Otherwise, we would have expected $\nabla \cdot \mathbf{B} = 0$ since $\mathbf{B}$ is defined as a curl. The singularity is a monopole for $\mathbf{B}$. The monopole also explains why it is impossible to define a gauge field $\mathbf{A}(\mathbf{b})$ without introducing a line of singularities, which will lie along some curve passing from the origin to infinity.

It clear that the Berry flux through the surface S will be unchanged if we deform the surface slightly ,so that it is no longer a perfect sphere. In fact, it will be unchanged as long as the surface does not pass through the singularity at $\mathbf{b} = 0$ during the course of the deformation. More generally, we can see that the Berry flux through a closed surface in $\mathbf{b}$-space will be equal to 0, if the surface does not enclose the origin, and is equal to 2π if the surface encloses the origin. We therefore say that the Berry flux is a topological invariant, which distinguishes surfaces that include the singular point at the origin from those that do not.

Later in this course, we shall consider Hamiltonians with a more complicated space of parameters than the single vector $\mathbf{b}$. We may also need to consider more complicated invariants than just the Berry flux through a closed surface in parameter space. However, the example of a two-level system will be a good starting point for understanding these more complicated situations.

There will be a problem on the first problem set that generalizes the Berry connection to the case of a TRI Hamiltonian with $\Theta^2 = -1$, where the eigenstates are all two-fold degenerate, and formulates gauge invariance in this case.

Additional remarks

In this course, we shall make use of the Berry's phase primarily to help classify the possible ground states of a time-independent many-particle Hamiltonian, so there will be no actual dynamics involved. However, the Berry phase also plays an important role in many dynamic problems where there is a large separation of time scales for different degrees of freedom. One example, which will appear on the first problem set, considers the motion of an ion in a uniform magnetic field. You will need to integrate out the fast moving electrons and come up with an effective Hamiltonian for the motion of center of mass. Including the Berry's phase from the adiabatic elimination of the electron degrees of freedom is necessary to find the correct equation of motion for the ion.

We mention, here, one additional point. If Hamiltonian of a system describes a collection of spinless particles in the absence of a magnetic field, then time-reversal invariance allows us to choose eigenfunctions

that are real. Then at least locally, $\mathbf{A} = -\mathrm{Im}\langle n|\partial_{\mathbf{R}}|n\rangle = 0$, as long as the eigenfunctions can also be chosen to be single-valued and smooth functions of $\mathbf{R}$. However, this may not always be possible, e.g. in cases where the domain of allowed $\mathbf{R}$ is not simply connected. An example may be given in a later homework.

Some additional relations between the Berry curvature and the spectrum of a Hamiltonian are derived in Bernevig's book.

The name of Sir Michael Berry has been attached to the phase concepts described above because of the influence of his article: M. V. Berry (1984), "Quantal Phase Factors Accompanying Adiabatic Changes", Proceedings of the Royal Society A 392 (1802), which described the issues involved in a very clear way, in a a quantum mechanical context. However, as Berry himself has pointed out, the basic concepts have a much longer history, some dating back to work by Darboux, in 1896. An important earlier reference is S. Pancharatnam (1956),"Generalized Theory of Interference, and Its Applications. Part I. Coherent Pencils", Proc. Indian Acad. Sci. A 44: 247262. Sometimes the Berry phase is referred to as the "Pancharatnam -Berry phase". More often, it is simply referred to as the "geometric phase." The importance of geometric phase as a way of characterizing integer quantized Hall states in a periodic potential was discussed by D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982), some time earlier than Berry's 1984 article.

The Landau-Zener Problem

A famous illustration of the predictions of the adiabatic theorem is the Landau-Zener problem, which was solved independently in 1932 by Landau, Zener, Stückelberg, and Majorana. The problem supposes a time-dependent 2×2 Hamiltonian given by

$$H = \Delta\sigma^x + \alpha(t/\tau)\sigma^z \tag{39}$$

over an infinite time interval $-\infty < t < \infty$. Assuming that the system is in the ground state at $t = -\infty$, which means $\sigma^z = 1$, if $\alpha > 0$, we may ask what is the probability P that the system is still in its ground state for $t \to +\infty$, which means that $\sigma^z = -1$ in this case. The result is

$$P = 1 - e^{-\pi\tau\Delta^2/\alpha}. \tag{40}$$

We see that the deviation from the adiabatic limit (P=1) falls of exponentially with τ, In the limit of large τ (slow passage), whereas $P \to 0, \propto \tau$, in the limit of fast passage. Since the Hamiltonian is real, we can choose a basis where the energy eigenstates are always real, so there is no Berry phase in this problem. There will, of course, be a dynamic phase, which depends on time.

Though the answer to the Landau-Zener problem is simple, the derivation is definitely not. The problem is discussed in many places, including ”Quantum Mechanics” by Landau and Lifshitz.