Advanced quantum mechanics
TD 1 : Adiabatic approximation and the Berry phase

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Consider a quantum system whose Hamiltonian $\hat{H}_t$ depends on time t. Let $\{|m_t\rangle\}$ be a complete set of eigenstates at time t :

$$\hat{H}_t \, |m_t\rangle = E_m(t) \, |m_t\rangle \ . \tag{1}$$

Note that $|m_t\rangle$ is an instantaneous eigenstate, *not* the state obtained by evolving $|m_0\rangle$ according to the Schrödinger equation. In particular, eigenstates belonging to different times need not be orthogonal. We assume that at time $t = 0$ the system is in a particular eigenstate $|n_0\rangle$. We will show that if the variation of $\hat{H}_t$ with time is sufficiently slow, the system remains in the instantaneous eigenstate $|n_t\rangle$ ("adiabatic evolution"). We wish to find the time-dependent phase factor that appears in front of $|n_t\rangle$.

1 Some useful relations

1. Use the normalization $\langle m_t|m_t\rangle = 1$ to show that $\langle m_t|\dot{m}_t\rangle$ is purely imaginary.
2. Show that for $l \neq m$:

$$\langle l_t| \, \dot{\hat{H}}_t \, |m_t\rangle = (E_m(t) - E_l(t)) \, \langle l_t|\dot{m}_t\rangle \ . \tag{2}$$

For $l = m$, the equation instead gives the Hellmann–Feynman relation

$$\langle m_t| \, \dot{\hat{H}}_t \, |m_t\rangle = \dot{E}_m(t) \ . \tag{3}$$

2 The adiabatic theorem

We decompose the state vector of the system at time t :

$$|\psi_t\rangle = \sum_m c_m(t) \, |m_t\rangle \ , \tag{4}$$

and we remind that $|\psi_0\rangle = |n_0\rangle$.

1. Show that the exact equations for $c_n(t)$ are

$$\dot{c}_n(t) = -\frac{iE_n(t)}{\hbar} c_n(t) - \sum_m c_m(t) \, \langle n_t|\dot{m}_t\rangle \ . \tag{5}$$

What approximation allows you to neglect transitions between different instantaneous eigenstates ?

2. To study transitions between instantaneous eigenstates, write the coefficients in the form

$$c_m(t) = b_m(t) \exp\left[-\frac{i}{\hbar}\int_0^t E_m(t') \, dt'\right] . \tag{6}$$

(a) Show that the equations for the slowly varying amplitudes $b_m(t)$ are

$$\dot{b}_m(t) = -\sum_l b_l(t) \, \langle m_t|\dot{l}_t\rangle \exp\left[\frac{i}{\hbar}\int_0^t \big(E_m(t') - E_l(t')\big) \, dt'\right] . \tag{7}$$

(b) Suppose that the system is initially in the instantaneous eigenstate $|n_0\rangle$:

$$b_n(0) = 1, \qquad b_{m\neq n}(0) = 0. \tag{8}$$

To first order in the transitions out of state n, show that, for $m \neq n$,

$$b_m(t) \simeq -\int_0^t dt' \, \langle m_{t'}|\dot{n}_{t'}\rangle \exp\left[\frac{i}{\hbar}\int_0^{t'} \big(E_m(t'') - E_n(t'')\big)\, dt''\right]. \tag{9}$$

(c) The phase appearing in the transition amplitude (9) is

$$\phi(t') = \frac{1}{\hbar}\int_0^{t'} \big(E_m(t'') - E_n(t'')\big)\, dt''. \tag{10}$$

Its rate of change is

$$\dot{\phi}(t') = \frac{E_m(t') - E_n(t')}{\hbar}. \tag{11}$$

Thus, when the energy difference is large, the phase changes rapidly with time. Contributions to the transition amplitude from different times then tend to cancel.

To make this explicit, consider for simplicity a time interval over which $\langle m_t|\dot{n}_t\rangle$ and the energy difference $E_m(t) - E_n(t)$ vary slowly. Denoting the energy difference by

$$\Delta E = E_m - E_n, \tag{12}$$

treat these quantities as approximately constant in the integral obtained in part (b).

Show that the magnitude of the resulting transition amplitude is of order

$$|b_m| \sim \frac{\hbar\,|\langle m|\dot{n}\rangle|}{|\Delta E|}. \tag{13}$$

What condition must therefore be satisfied for transitions to remain small ?

Finally, using the result of Section 1, show that this condition can be written as

$$\frac{\hbar\,|\langle m_t|\dot{H}(t)|n_t\rangle|}{|E_m(t) - E_n(t)|^2} \ll 1\ . \tag{14}$$

This is the adiabaticity condition.

3. Consider following example : a localized electron (with spin-1/2) in a time-dependent magnetic field,

$$\vec{B}(t) = B_0\vec{u}_z + B_1(t)\vec{u}_x\ , \tag{15}$$

evolving from initial time t_i to final time t_f such that

$$B_1(t_i) < 0 \quad \text{and} \quad |B_1(t_i)| \gg B_0\ , \tag{16}$$

$$B_1(t_f) > 0 \quad \text{and} \quad |B_1(t_f)| \gg B_0\ . \tag{17}$$

(a) Write the Hamiltonian in the $\{|+\rangle_z, |-\rangle_z\}$ basis.

(b) Find the energy eigenvalues $E_\pm$ (with E_- being the lower eigenvalue). Hint : choose a continuous angle $\theta \in (-\pi/2, \pi/2)$ defined by $\cos\theta(t) = \frac{B_0}{|B(t)|}$ and $\sin\theta(t) = \frac{B_1(t)}{|B(t)|}$. Extra : show that with a convenient real phase convention the corresponding eigenvectors are

$$|E_+\rangle \;=\; \cos\frac{\theta}{2}\,|+_z\rangle + \sin\frac{\theta}{2}\,|-_z\rangle\ , \tag{18}$$

$$|E_-\rangle \;=\; -\sin\frac{\theta}{2}\,|+_z\rangle + \cos\frac{\theta}{2}\,|-_z\rangle\ . \tag{19}$$

(c) Assume that the system is initially in the excited state $|-\rangle_x$. (Note that the electron has a negative gyromagnetic ratio, and the excited state is thus the spin state parallel to $\vec{B}$.) We wish to find the condition for the system to stay in the excited state during the evolution, and thus to finish in the state $|+\rangle_x$ at time t_f. First find the condition for $\dot{\theta}$, and then for $\dot{B}_1(t)$. Introduce a characteristic time scale T over which the transverse field $B_1(t)$ changes by an amount comparable to the longitudinal field B_0. Formulate your condition in terms of this time scale. Interpret your result.

3 The Berry phase (Proc. Roy. Soc. Lond. A392, 45-57 (1984))

Suppose now that the Hamiltonian depends implicitly on time via a real vector $\vec{\rho}$: $\hat{H} = \hat{H}(\vec{\rho})$ with $\vec{\rho} = \vec{\rho}(t)$. As an example, we can consider again a spin $\vec{s}$ in a changing magnetic field $\vec{B}(t)$:

$$\hat{H} = -\gamma \hat{\vec{s}} \cdot \vec{B}(t) \ , \tag{20}$$

with $\gamma = -\frac{ge}{2m_e} = -\frac{g\mu_B}{\hbar}$ gyromagnetic ratio for the electron. In this case the vector $\vec{\rho}$ corresponds to the magnetic field.
Let the initial state be $|n(\vec{\rho}_0)\rangle$ and assume that the adiabatic approximation is valid, such that the state vector takes the form

$$|\psi_t\rangle = c_n(t)\, |n(\vec{\rho}_t)\rangle \ . \tag{21}$$

We wish to determine the coefficient $c_n(t)$, once a phase convention for the instantaneous eigenstates has been chosen.

4. Show that $c_n(t)$ can be written as

$$c_n(t) = e^{i\phi_n(t)} e^{i\gamma_n(t)} \tag{22}$$

where

(a) $\phi_n(t)$ involves the energies $E_n(t')$ for $0 < t' < t$ (the dynamical phase).

(b) $\gamma_n(t)$ is defined as

$$\dot{\gamma}_n(t) = i \langle n(\vec{\rho}_t)| \left[\vec{\nabla}_{\vec{\rho}} |n(\vec{\rho}_t)\rangle\right] \cdot \dot{\vec{\rho}}_t \tag{23}$$

$$\gamma_n(0) = 0 \tag{24}$$

5. In what follows we assume that the variable $\vec{\rho}_t$ follows a closed path C in the parameter space. We consider thus a cyclic evolution around the closed path C such that $\vec{\rho}_T = \vec{\rho}_0$. Consider the *geometric phase* accumulated during this cyclic evolution in a time T. Write it in the form

$$\gamma_n(C) = i \oint_C \langle n(\vec{\rho})| \left[\vec{\nabla}_{\vec{\rho}} |n(\vec{\rho})\rangle\right] \cdot d\vec{\rho} \, , \tag{25}$$

which is the *closed-path Berry phase*. Argue that this accumulated geometric phase is independent of the rate at which the path is traversed, provided the evolution remains adiabatic.

One also introduces the (gauge-dependent [1]) Berry connection or Berry potential :

$$\vec{\mathcal{A}}_n(\vec{\rho}) = i \langle n(\vec{\rho})| \vec{\nabla}_{\vec{\rho}} |n(\vec{\rho})\rangle \tag{26}$$

so the Berry phase can be written terms of the Berry connection :

$$\gamma_n(C) = \oint_C \vec{\mathcal{A}}_n(\vec{\rho}) \cdot d\vec{\rho}\,. \tag{27}$$

6. Use Stokes' theorem to express $\gamma_n(C)$ in terms of the (gauge-invariant) *Berry curvature* $\vec{\mathcal{F}}_n(\vec{\rho}) = \vec{\nabla}_{\vec{\rho}} \times \vec{\mathcal{A}}_n(\vec{\rho})$.
7. Now obtain

$$\gamma_n(C) = -\int\int_S d\vec{S} \cdot \vec{V}_n(\vec{\rho})\,, \tag{28}$$

where the surface S is enclosed by C and

$$\vec{V}_n(\vec{\rho}) = \mathrm{Im}\left(\left[\vec{\nabla}_{\vec{\rho}} \langle n(\vec{\rho})|\right] \times \left[\vec{\nabla}_{\vec{\rho}} |n(\vec{\rho})\rangle\right]\right)\,. \tag{29}$$

Useful relation : $\vec{\nabla} \times (f\vec{A}) = f\vec{\nabla} \times \vec{A} + (\vec{\nabla} f) \times \vec{A}$.

8. Assume that there is no degeneracy of the states on this surface and smooth dependence on $\vec{\rho}$. Start from the instantaneous eigenvalue equation and show that

$$\vec{\nabla}_{\vec{\rho}} |n(\vec{\rho})\rangle = \sum_{m \neq n} |m(\vec{\rho})\rangle \frac{\langle m(\vec{\rho})| \left(\vec{\nabla}_{\vec{\rho}} H(\vec{\rho})\right) |n(\vec{\rho})\rangle}{E_n(\vec{\rho}) - E_m(\vec{\rho})} - i\,|n(\vec{\rho})\rangle\, \vec{\mathcal{A}}_n(\vec{\rho}) \tag{30}$$

with $\vec{\mathcal{A}}_n(\vec{\rho})$ the Berry connection.

9. Use Eq. (30) to show that

$$\vec{V}_n(\vec{\rho}) = \mathrm{Im}\left(\sum_{m \neq n} \frac{\langle n(\vec{\rho})| \left[\vec{\nabla}_{\vec{\rho}} H\right] |m(\vec{\rho})\rangle \times \langle m(\vec{\rho})| \left[\vec{\nabla}_{\vec{\rho}} H\right] |n(\vec{\rho})\rangle}{(E_m - E_n)^2}\right) \tag{31}$$

10. Now consider again the case of a spin $\vec{s}$ in a slowly varying magnetic field $\vec{B}$. If the initial state is $|s, s_{z_B} = m_s\rangle \equiv |m_s\rangle$ (this is an eigenstate of $\hat{\vec{s}}$ in the direction along the initial $\vec{B}$), show that one has

$$\vec{V}_{m_s}(\vec{B}) \;=\; \frac{1}{B^2}\,\mathrm{Im} \sum_{m \neq m_s} \frac{\langle m_s|\, \hat{\vec{s}}\, |m\rangle \times \langle m|\, \hat{\vec{s}}\, |m_s\rangle}{\hbar^2 (m - m_s)^2} \tag{32}$$

11. Then show that

$$\vec{V}_{m_s}(\vec{\rho} = \vec{B}) = m_s \frac{\vec{B}}{|\vec{B}|^3}\,. \tag{33}$$

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1. Under the gauge transformation

$$|n(\vec{\rho})\rangle \;\mapsto\; e^{i\chi(\vec{\rho})}\, |n(\vec{\rho})\rangle,$$

the Berry connection transforms as

$$\vec{\mathcal{A}}_n(\vec{\rho}) \;\mapsto\; \vec{\mathcal{A}}_n(\vec{\rho}) - \vec{\nabla}_{\vec{\rho}} \chi(\vec{\rho})\,,$$

in direct analogy with the electromagnetic vector potential.

Hint : to evaluate the matrix elements $\langle m_s|\,\hat{\vec{s}}\,|m\rangle$ temporarily rotate the axes so that the z-axis points along $\vec{B}$. We also remind the standard relations

$$(\hat{s}_x + i\hat{s}_y)\,|s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s+1)}\,|s, m_s+1\rangle \ , \tag{34}$$

$$(\hat{s}_x - i\hat{s}_y)\,|s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s-1)}\,|s, m_s-1\rangle \ , \tag{35}$$

$$\hat{s}_z\,|s, m_s\rangle = \hbar m_s\,|s, m_s\rangle \ . \tag{36}$$

12. Derive from this a relation between the geometric phase $\gamma_{m_s}(C)$ and the solid angle $\Omega(C)$ subtended at the origin by the closed path of $\vec{B}$.
13. Consider a 2π rotation of $\vec{B}$ along a great circle, i.e. a rotation through 2π in a plane. What phase factor is obtained for integer-spin and half-integer-spin states ?

4 Experimental observation of the Berry phase

It might not be immediately clear that the Berry phase can be observed, since the expectation value of any observable is independent of the overall phase of a state. As usual, an interference experiment is needed to make a relative phase observable. Several experiments have confirmed the Berry-phase predictions. We briefly discuss one historic example here.

In 1987, Bitter and Dubbers observed the Berry phase using polarized neutrons in a magnetic field (Phys. Rev. Lett. **59**, 251 (1987)). A neutron beam was split into two paths, each sent through a region where the magnetic field direction varies slowly enough for the neutron spin to follow it adiabatically. Recombining the two paths produces an interference pattern that depends on the relative phase accumulated along each path. Since both paths involve the same dynamical phase (same field magnitude and travel time), the shift in the interference pattern isolates the geometric (Berry) contribution.

Concretely, a slow ($v \simeq 500\ \mathrm{m\,s^{-1}}$) beam of neutrons, polarized along an axis perpendicular to the beam direction z, travels through a cylinder carrying a helical magnetic field : a constant longitudinal component B_z and a transverse component B_1 that completes one right-handed turn of 2π around the cylinder axis. In the spin's rest frame, this is exactly the adiabatic circuit of Section 3 : the field vector $\vec{B}(t)$ traces a closed cone of half-angle $\theta = \arctan(B_1/B_z)$ around the z-axis, enclosing a solid angle Ω that depends only on the ratio B_z/B_1. Combining Eqs (28) and (33) then predicts a Berry phase $\gamma_{\pm 1/2} = \mp\frac{1}{2}\Omega$ for the two spin states, so that the *difference* directly measured in the interference signal is $\gamma_{-1/2} - \gamma_{1/2} = \Omega$.

Figure 1 compares this measured phase difference to the geometrically computed solid angle $\Omega(B_z/B_1)$, showing good agreement with the adiabatic prediction (small deviations at low B_z/B_1 arise because the adiabaticity condition is not yet well satisfied there).

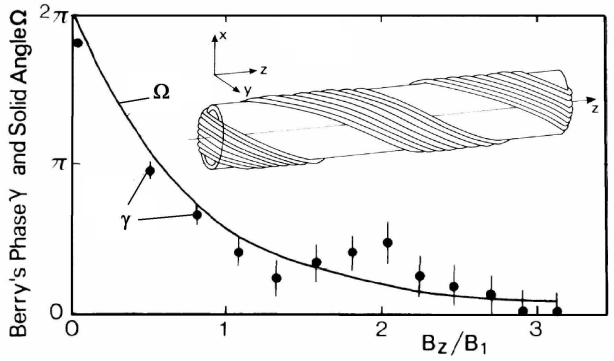


FIGURE 1 – Measurement of the Berry phase of neutrons. The inset shows the helical-field coil ; the neutron beam travels along z (coil length 40 cm, diameter 8 cm) ; an axial coil (not shown) produces the field B_z. The curve shows the Berry phase difference $\gamma_{-1/2} - \gamma_{1/2}$ together with the solid angle Ω, as a function of B_z/B_1. From Phys. Rev. Lett. **59**, 251 (1987).