

# SLOW PROCESSES IN Q. MECHANICS

This is a topic of v. considerable subtlety, with many results only found in the last 10-20 years, and many problems still outstanding. The problem is inherently non-perturbative, and the results are of enormous theoretical importance, not just in ordinary QM; they form part of the whole underpinning of quantum field theory, both in its relativistic form & in its application to condensed matter systems.

We begin with a review of elementary results in the adiabatic limit, including the derivation of geometric phases, the Born-Oppenheimer approximation, and the Landau-Dykhne formulae. We then continue with a discussion of the path integral formulation of these results, in preparation for a systematic treatment of deviations from the results in the adiabatic limit. This can be done in a systematic expansion in powers of a "slowness parameter", suggesting a renormalization procedure; but the expansion is intrinsically divergent and the non-perturbative character quickly becomes apparent. The problem raises quite interesting general questions in the theory of asymptotic expansions, as well as having important implications for the theory of effective Hamiltonians and effective Lagrangians.

## 1. ELEMENTARY RESULTS

The following results are considered to be basic to the whole subject. Even so, they are all rather subtle - thus, although elementary, they are by no means simple. We begin by recalling, without extensive derivation, the results of elementary time-dependent perturbation theory, and then consider the adiabatic limit of 1-particle QM. This leads to the idea of geometric phase, and the Born-Oppenheimer approx. We then review the basic "Landau-Dykhne" theory of transitions in this limit, finishing with a brief geometric discussion of the whole picture in both Hamiltonian space and Hilbert space.

1. (a) TIME-DEPENDENT PERTURBATION THEORY: This is a topic to be found in every book on Q.M.; however it conceals some interesting features.

We begin with the time-dependent Schrödinger eqn., in the form

$$H(t)\psi(t) = i\hbar\partial_t\psi(t) \quad (1)$$

Now we can consider 2 obvious approximation schemes for this Hamiltonian. One obtains if the time-dependent part of  $H(t)$  is small; and the other applies if there is a clear separation of time-scales, i.e., if the time-dependence is either very slow or very fast, compared to the characteristic timescales in the static part of the Hamiltonian. We look at these in turn.

(i) Weak Perturbation: The simplest case, at first glance, is that of a weak perturbation. We write the Hamiltonian as

$$H = H_0 + V(t) \quad (2)$$

and assume

$$H_0 |\phi_n\rangle = \epsilon_n^0 |\phi_n\rangle \quad (3)$$

Then, in a sense to be specified, the perturbation  $V(t)$  will be assumed small compared to  $H_0$ . Thus we begin by writing things in terms of the  $\phi_n$ , which satisfy the time-dependent equation

$$\hat{H}_0 \phi_n(t) = i\hbar \partial_t \phi_n(t) \quad (4)$$

We assume a solution  $\psi(t)$  of the full Schrödinger eqn (1) in the form of a sum over the  $\phi_n$ :

$$\psi(t) = \sum_n a_n(t) \phi_n(t) \quad (5)$$

where

$$\phi_n(t) = \phi_n e^{-i/\hbar \epsilon_n^0 t} \quad (6)$$

Substituting (5) in (1), we find

$$\left. \begin{aligned} \sum_n a_n(t) [(H_0 - i\hbar \partial_t) + V(t)] \phi_n(t) - i\hbar \sum_n \dot{a}_n(t) \phi_n(t) \\ = \sum_n [a_n(t) V(t) \phi_n(t) - i\hbar \dot{a}_n(t) \phi_n(t)] = 0 \end{aligned} \right\} (7)$$

so, taking the inner product with  $\phi_m^\dagger(t)$ , we have

$$\dot{a}_n(t) = -i/\hbar \sum_m V_{nm}(t) a_m(t) \quad (8)$$

This result is exact. From (6), we may also write it as

$$\dot{a}_n(t) = -i/\hbar \sum_m \bar{V}_{nm}(t) a_m(t) e^{i/\hbar (\epsilon_n^0 - \epsilon_m^0) t} \quad (9)$$

where  $\bar{V}_{nm}(t) = \langle \phi_n | V(t) | \phi_m \rangle$ . We note that  $\bar{V}_{nm}(t)$  still depends on  $t$ , through the time dependence of  $V(t)$  itself. Now

this equation is less simple than it looks at first glance - if the  $\bar{V}_{nm}(t)$  are not small, we have a set of  $N$  coupled 1st-order differential equations, with  $t$ -dependent coefficients, and no hope of solution.

Accordingly we assume that  $V(t) \rightarrow \lambda V(t)$  (10)

where in the 1st instance we assume  $\lambda \ll 1$ ; this allows a perturbative expansion. We write

$$a_n(t) = \sum_{k=0}^{\infty} \lambda^k a_n^{(k)}(t) = a_n^{(0)} + \lambda a_n^{(1)}(t) + \lambda^2 a_n^{(2)}(t) + \dots$$
 (11)

so that as  $\lambda \rightarrow 0$ , the system stays in one of the stationary states, i.e.,  $a_n(t) \rightarrow a_n^{(0)}$ , a time-independent constant.

Equating powers of  $\lambda$ , after substituting (11) into (9), we find

$$\dot{a}_n^{(k+1)}(t) = -\frac{i}{\hbar} \sum_m a_m^{(k)}(t) V_{nm}(t) \equiv -\frac{i}{\hbar} \sum_m a_m^{(k)}(t) \bar{V}_{nm}(t) e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t}$$
 (12)

Below we develop a systematic perturbative expansion in  $\lambda$ . First we recall the result for  $\lambda \ll 1$ , when it suffices to go to 1st order in  $\lambda$ . We then have

$$\dot{a}_n^{(1)}(t) = -\frac{i}{\hbar} \sum_m a_m^{(0)} \bar{V}_{nm}(t) e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t}$$
 (13)

from which we have

$$a_n^{(1)}(t) = -\frac{i}{\hbar} \sum_m a_m^{(0)} \int dt' \bar{V}_{nm}(t') e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t'}$$
 (14)

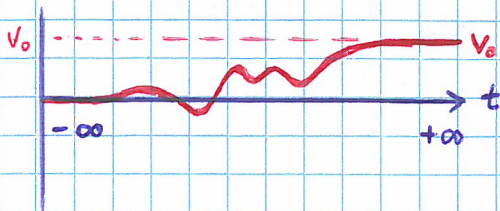
This eqn., valid only for  $\lambda \ll 1$ , is often used to analyze problems in which an external AC field is treated classically (i.e., as a scalar function  $V(t)$ ).

It is also employed in problems where  $V(t)$  is switched on from zero to a finite value, so that

$$V(t) \xrightarrow{t \rightarrow -\infty} 0 \quad V(t) \xrightarrow{t \rightarrow \infty} V_0$$
 (15)

In this case the integral in (14) is apparently undefined; however this pathology disappears if we integrate by parts:

$$\begin{aligned}
 a_n^{(1)}(t) &= -\frac{i}{\hbar} \sum_m a_m^{(0)} \int_{-\infty}^t dt' \bar{V}_{nm}(t') e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t'} \\
 &= \sum_m \left\{ a_m^{(0)} \int_{-\infty}^t dt' \frac{\partial \bar{V}_{nm}(t')}{\partial t'} \frac{e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t'}}{\epsilon_n^0 - \epsilon_m^0} \right. \\
 &\quad \left. - \left[ \bar{V}_{nm}(t') \frac{e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t'}}{\epsilon_n^0 - \epsilon_m^0} \right]_{-\infty}^t \right\} \quad (16)
 \end{aligned}$$



To understand the meaning of these terms, we note (see left) that the 2nd definite integral arises purely from the time-dependence of the shifted state when  $t \rightarrow \infty$ ;

recall we were assuming (15) at  $t \rightarrow \infty$ .

It is thus conventional to ignore the 2nd term when discussing the  $t \rightarrow \infty$  limit, since it is simply equal to the time dependence of the state  $\phi_n(t)$  coming from the shift in energy caused by switching on  $V_0$ ; from time-INDEPENDENT perturbation theory we have

$$\phi_n = \sum_m' \phi_m \frac{V_{nm}^0}{\epsilon_n^0 - \epsilon_m^0} \quad (17)$$

so that the 2nd term in (16) is just the time-dependent contribution to  $\phi_n(t)$  coming from the energy shift in (17). It is thus the 1st term in (16) that is describing real transitions. Thus one often writes the TRANSITION PROBABILITY in the  $t \rightarrow \infty$  limit as

$$P_{nm} = \lim_{t \rightarrow \infty} |a_n^{(1)}(t)|^2 = \frac{1}{(\epsilon_n^0 - \epsilon_m^0)^2} \left| \int_{-\infty}^{\infty} dt' \frac{\partial V_{nm}(t')}{\partial t'} e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t'} \right|^2 \quad (18)$$

which makes clear that it is the time-varying part of the perturbation that is causing transitions.

(ii) PERTURBATION EXPANSION for GREEN FUNCTION : One can put the results in

eqns (11) and (12) in a much more compact form by simply inserting to form a complete series expansion. Rather than writing this for the coefficients themselves, it is more sensible & compact to simply give

the series expansion for the propagator of the system. Accordingly we go back to the basic expression for the propagator of the system, written in operator form as

$$\hat{G}(t, t') = \hat{G}^0(t, t') - \frac{i}{\hbar} \int_{t'}^t dt \hat{G}^0(t, \tau) \hat{V}(\tau) \hat{G}(\tau, t') \quad (19)$$

which when sandwiched between the states  $|\phi_n\rangle = |n\rangle$  and  $|\phi_m\rangle$  is just

$$G_{nm}(t, t') = G_n^0(t, t') \delta_{nm} - \frac{i}{\hbar} \int_{t'}^t dt G_n^0(t, \tau) V_{nm}(\tau) G_m(\tau, t') \quad (20)$$

Apart from this Dyson eqn, it is also pedagogically useful to also consider the equivalent integral equation for the time evolution operator  $U(t, t')$ , which in the interaction representation takes the form

$$\hat{U}(t, t') = \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t'}^t dt \hat{V}(\tau) \right\} \quad (21)$$

ie, which solves

$$\hat{V}(t) \hat{U}(t, t') = i\hbar \partial_t \hat{U}(t, t')$$

Both of these eqns (19) and (21) can be developed as formal power series expansions. The time evolution operator is straightforward; the time-ordered expansion of (21) gives

$$\begin{aligned} \hat{U}(t, t') &= 1 - \frac{i}{\hbar} \int_{t'}^t dt \hat{V}(\tau) \hat{U}(\tau, t') \\ &= 1 - \frac{i}{\hbar} \int_{t'}^t dt_1 \hat{V}(\tau_1) + \left(\frac{i}{\hbar}\right)^2 \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 \hat{V}(\tau_1) \hat{V}(\tau_2) + \dots \\ &\equiv 1 - \sum_{k=1}^{\infty} \left(\frac{-i}{\hbar}\right)^k \prod_{r=1}^k \int_{t'}^{t_{r+1}} dt_r \hat{V}(\tau_r) \end{aligned} \quad (22)$$

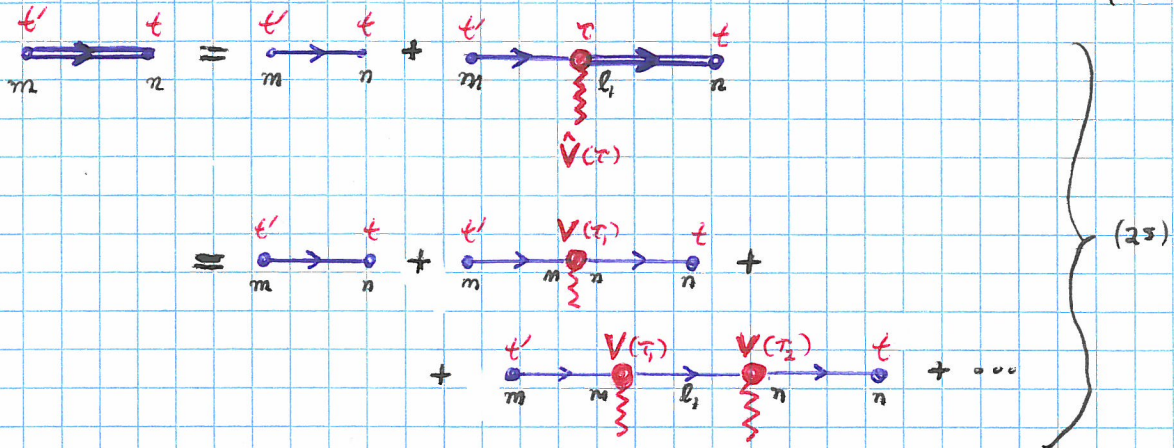
In the same way, the Green function can be expanded as

$$\begin{aligned} \hat{G}(t, t') &= \hat{G}^0(t, t') - \frac{i}{\hbar} \int_{t'}^t dt_1 G^0(t, \tau_1) V(\tau_1) G^0(\tau_1, t') \\ &\quad + \left(\frac{-i}{\hbar}\right)^2 \int_{t'}^t dt_1 \int_{t'}^{\tau_1} dt_2 G^0(t, \tau_1) V(\tau_1) G^0(\tau_1, \tau_2) V(\tau_2) G^0(\tau_2, t') \\ &\quad + \dots \end{aligned} \quad (23)$$

which is more involved than (22) [the expansion (22) is so simple

just because we work in the interaction representation]. If we wish to write a compact expression for this series, we can do this so

$$\hat{G}(t, t') = G_0(t, t') + \sum_{k=1}^{\infty} \left(\frac{-i}{\hbar}\right)^k \prod_{r=1}^k \left[ \int_{t'}^{t_{r-1}} dt_r \delta(t - t_r) G_0(t_{r-1}, t_r) V(t_r) \right] G_0(t_r, t') \quad (24)$$



If we sandwich these terms between eigenstates  $|\Phi_m\rangle$  of  $H_0$ , then we have

$$G_{nm}(t, t') = G_{nm}^0(t, t') + \sum_{k=1}^{\infty} \left(\frac{-i}{\hbar}\right)^k \prod_{r=1}^k \left[ \int_{t'}^{t_{r-1}} dt_r \sum_{l_r} \delta(t - t_r) \delta_{nl_r} G_0(t_{r-1}, t_r) V_{l_r}(t_r) \right] \times G_m^0(t_r, t') \quad (26)$$

$$= G_{nm}^0(t, t') - \frac{i}{\hbar} \int_{t'}^t dt_1 G_n^0(t, t_1) V_{nm}(t_1) G_m^0(t_1, t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 \sum_{l_1} G_n^0(t, t_1) V_{nl_1}(t_1) G_{l_1}^0(t_1, t_2) V_{l_1 l_2}(t_2) G_m^0(t_2, t') + \dots \quad (27)$$

We can make the sort of expansion in the eigenstate basis for (22). Notice that the lowest order (in  $V(t)$ ) truncation of (27) just gives

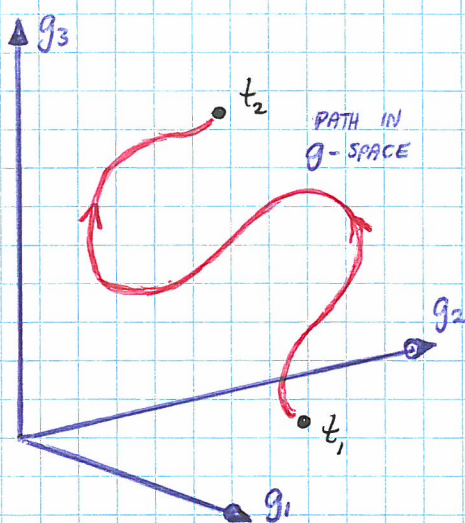
$$G_{nm}^{(1)}(t, t') = G_{nm}^0(t, t') - \frac{i}{\hbar} \int_{t'}^t dt_1 G_n^0(t, t_1) V_{nm}(t_1) G_m^0(t_1, t') = G_{nm}^0(t, t') - \frac{i}{\hbar} \int_{t'}^t dt_1 V_{nm}(t_1) e^{i/\hbar(\epsilon_n^0 - \epsilon_m^0)t_1} \quad (28)$$

which corresponds to the lowest-order result (14).

Formally, these expansions are still perturbative, and subject to all the limitations of perturbation expansions. In old-style perturbative developments of quantum field theory, equations (22) and (23) played a central role.

## 1.(b) ADIABATIC LIMIT & BERRY PHASE

Let us now consider a more general approach to the adiabatic limit. We begin by writing the Hamiltonian in the form



$$\left. \begin{aligned} \mathcal{H}(t) &= \mathcal{H}_0 + V(t) \\ &= \mathcal{H}(g(t)) \end{aligned} \right\} \quad (29)$$

where we parametrize the Hamiltonian now by a set of couplings

$$\underline{g}(t) = (g_1(t), g_2(t), \dots, g_N(t)) \quad (30)$$

so that the Hamiltonian is now

$$\mathcal{H}(\underline{g}) = \mathcal{H}_0 + \sum_{n=1}^N g_n \hat{O}_n \quad (31)$$

and where the  $\hat{O}_n$  are operators acting in the Hilbert space of the system. Then, as we vary the time  $t$ , the system follows a path in "Hamiltonian space", i.e., the space of couplings  $\{g_m\}$ . This is shown in the diagram above, in the case where  $g$  has 3 components. We imagine the system starting at  $t=t_1$  and finishing at  $t=t_2$ .

(i) QM IN ADIABATIC REGIME: First consider the slow regime (i.e., without yet going to the limit). We can then define, in the standard way, a set of adiabatic states as

$$\mathcal{H}(\underline{g}) \phi_n(\underline{g}) = E_n(\underline{g}) \phi_n(\underline{g}) \quad (32)$$

The wave-function of the system at time  $t$  will then be

$$\psi(t) = \sum_n c_n(t) \phi_n(g(t)) e^{-i/\hbar \int dt' E_n(g(t'))} \quad (33)$$

and  $\psi(t)$  obeys

$$\mathcal{H}(t) \psi(t) = i\hbar \partial_t \psi(t) \quad (34)$$

If we now substitute (33) into (34), we have

$$\begin{aligned} \mathcal{H}(t) \psi(t) &= \sum_n c_n(t) E_n(g(t)) \phi_n(g(t)) e^{-i\hbar^{-1} \int dt' E_n(g(t'))} \\ &= \sum_n \left\{ i\hbar \left[ \dot{c}_n(t) \phi_n(g(t)) + c_n(t) \partial_t \phi_n(g(t)) \right] \right. \\ &\quad \left. + c_n(t) E_n(g(t)) \phi_n(g(t)) \right\} e^{-i\hbar^{-1} \int dt' E_n(g(t'))} \end{aligned} \quad (35)$$

so that we have the interesting result that

$$\sum_n \left[ \dot{c}_n(t) \phi_n + c_n(t) \partial_t \phi_n \right] e^{-i\hbar^{-1} \int dt' E_n(t')} = 0 \quad (36)$$

If we multiply this on the left by  $\langle m(t) | = \phi_m^*(g(t))$ , then we immediately find that

$$\begin{aligned} \dot{c}_m(t) &= - \sum_n \langle m | \partial_t n \rangle c_n(t) e^{-i\hbar^{-1} \int dt' (E_n(t') - E_m(t'))} \\ &\equiv i \sum_n \underline{A}_{mn}(g(t)) \cdot \dot{g}(t) c_n(t) e^{-i\hbar^{-1} \int dt' (E_n(t') - E_m(t'))} \end{aligned} \quad (37)$$

for  $m \neq n$ , where we define a quantity

$$\begin{aligned} \underline{A}_{mn}(g) &= i \langle m | \partial_g n \rangle \\ &\equiv i \langle \phi_m(g) | \nabla_g | \phi_n(g) \rangle \end{aligned} \quad (38)$$

which we will see later can be thought of as a "gauge potential" in the space of Hamiltonians. For  $m=n$ , we get the simple result

$$\begin{aligned} \dot{c}_n(t) &= - \langle n | \partial_t n \rangle c_n(t) \\ &= i \underline{A}_{nn}(g) \cdot \dot{g}(t) c_n(t) \end{aligned} \quad (39)$$

So far these results are quite general, and have nothing to do with the adiabatic regime. However we now define this limit a little more precisely. There are a number of ways of doing this; for example

(1) We define all timescales in terms of a characteristic time for the system in question. This timescale  $\tau_0$  will typically be the inverse (in units of  $\hbar$ ) of a characteristic energy  $E_0$ , which is often the level distance between the ground state energy and that of the first excited state (but this is



certainly not always the case). Then the adiabatic regime corresponds to

$$t\epsilon_0 \equiv t/T_0 \gg 1 \quad (\text{adiabatic regime}) \quad (40)$$

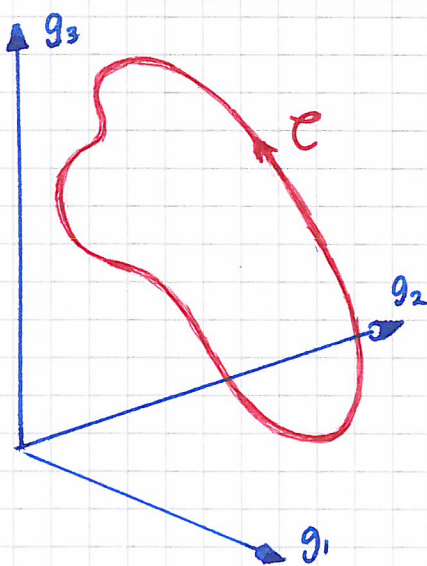
and the adiabatic limit is  $t\epsilon_0 \rightarrow \infty$ .

(ii) Another definition simply consists in defining a time scaling factor  $\epsilon$ , which is used in all equations. Thus, we "stretch" time, by defining

$$\left. \begin{aligned} \epsilon t &= \bar{t} \\ t &= \bar{t}/\epsilon \end{aligned} \right\} \quad (41)$$

and the adiabatic regime is defined by  $\epsilon \ll 1$ ; the adiabatic limit is then  $\epsilon \rightarrow 0$ . This definition is less precise than the first one.

(ii) BERRY PHASE & FLUX IN g-SPACE : We now follow the



interesting argument of Berry (which was anticipated by chemists like Longuet-Higgins, Mead & Truhler) and consider what happens when we transport a Hamiltonian adiabatically around a closed path in Hamiltonian space. The situation is as shown at left - we assume

$$\left. \begin{aligned} H(t) &= H(g(t)) \\ g(T) &= g(0) \\ T &\rightarrow \infty \end{aligned} \right\} \quad (42)$$

The 1st of these eqns makes the parameters  $g = (g_1, \dots, g_n)$  time-dependent; the 2nd eqn. assures we

take the system through a closed circuit between times  $t=0$  and  $t=T$ . The 3rd condition takes us to the adiabatic limit.

We define the instantaneous eigenstates as in (32). Then the "quantum adiabatic theorem" tells us that unless there is a level-crossing in the system, the system will, if it starts at  $t=0$  in the state  $|n\rangle \equiv |\phi_n\rangle$ , then it must finish at  $t=T$  in the same state  $|n\rangle$ . The meaning & derivation of this theorem can be found from eqns. (37) & (39). If we let  $\dot{g}(t) \rightarrow 0$  in these 2 eqns, then we go to the adiabatic limit. Let us now consider first the fate of state  $|n\rangle$  during this circuit - this is the question addressed by Berry (in the next subsection we consider the time evolution of the states  $|m\rangle$ , for  $m \neq n$ ).

From eqns (33) and (39), we see immediately that the state of the system after a time  $t$  can be written as

$$\psi(t) = |n(g(t))\rangle e^{-i\Phi_n(t)} \quad (43)$$

where

$$\Phi_n(t) = \phi_n(t) + \gamma_n(t) \quad (44)$$

with

$$\phi_n(t) = \frac{1}{\hbar} \int_0^t dt' E_n(g(t')) \quad (45)$$

$$\gamma_n(t) = i \int_0^t dt' \dot{g}(t') \langle n(g(t')) | \nabla_g n(g(t')) \rangle \quad (46)$$

$$\text{i.e. } \gamma_n(t) = \int_{g(0)}^{g(t)} dg \cdot \underline{A}_{nn}(g) \equiv \int dt' \dot{g}(t') \cdot \underline{A}_{nn}(g(t'))$$

Now let's consider the result of taking the system through a circuit. We see that the following result obtains after a time  $t$ :

(a) The dynamical phase  $\phi_n(T) = \frac{1}{\hbar} \int_0^T dt' E_n(g(t'))$  accumulates. In a certain rather special sense we can think of this phase as a "clock" - it has measured the total time  $T$  (in units  $\hbar/E_n(t')$ , which we note vary round the circuit). Thus as  $T \rightarrow \infty$ , so does  $\phi_n(T)$ .

(b) The geometrical or "Berry" phase  $\gamma_n(T)$ , which is the integral of (46) round the circuit  $C$ . To see its geometric significance, define the quantity

$$\underline{B}_n(g) = \nabla_g \times \underline{A}_{nn}(g) \quad (47)$$

which we can think of as an analogue to the EM field  $\underline{B}(r)$  defined in real space. From (39) we see that  $\underline{A}_{nn}(g)$  must be real (since  $\langle n | \partial_t n \rangle$  must be imaginary;  $\dot{c}_n$  is orthogonal to  $\underline{c}_n$ ). It then follows we can also write

$$\begin{aligned} \underline{B}_n(g) &= g_m (\nabla_g \times \langle n | \nabla_g n(g) \rangle) \\ &= g_m \langle \nabla_g n(g) | \times | \nabla_g n(g) \rangle \end{aligned} \quad (48)$$

Now from (46) we clearly have

$$\gamma_n(T) = \oint_C dg \cdot \underline{A}_{nn}(g) = \oint_{S_C} d\underline{S}_g \cdot \underline{B}_n(g) \quad (49)$$

where the curve  $\mathcal{C}$  bounds the surface  $S_{\mathcal{C}}$  in  $g$ -space. The quantity  $\mathcal{L}_n(g)$  thus represents a kind of field, and  $\gamma_n$  we now see represents a "flux" through this surface, i.e., we have

$$\gamma_n(T) \xrightarrow{T \rightarrow \mathcal{C}} \gamma_n(\mathcal{C}) \tag{50}$$

i.e.,  $\gamma_n(\mathcal{C})$  depends only on the contour followed. Notice here that  $\gamma_n(\mathcal{C})$  as a quantity does NOT depend on  $\hbar$ , i.e., it is not necessarily even quantum-mechanical!

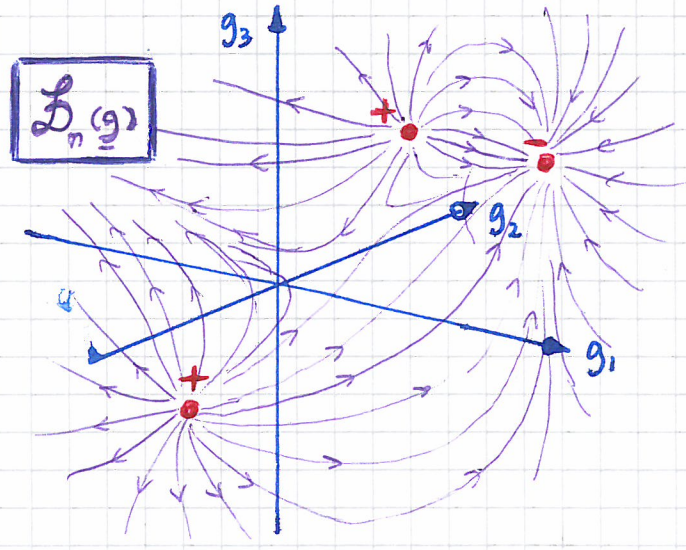
Obviously we would like to get a feeling for how the fields  $\hat{A}_m(g)$  and  $\mathcal{L}_n(g)$  behave in  $g$ -space. To do this, let us first note that for 2 states  $|m(g)\rangle$  and  $|n(g)\rangle$ , the following identity is easily proved:

$$\langle m(g) | \nabla_g n(g) \rangle = \frac{\langle m(g) | \nabla_g \hat{H}(g) | n(g) \rangle}{E_n(g) - E_m(g)} \tag{51}$$

Then, by inserting intermediate states  $|m\rangle$  into (48), we immediately get

$$\mathcal{L}_n(g) = \sum_{m \neq n} \frac{\langle n(g) | \nabla_g \hat{H}(g) | m(g) \rangle \times \langle m(g) | \nabla_g \hat{H}(g) | n(g) \rangle}{(E_n(g) - E_m(g))^2} \tag{52}$$

This formula immediately makes it clear where the "sources" of the field  $\mathcal{L}_n(g)$  lie in  $g$ -space; they come from OTHER LEVELS - and in particular, from degeneracy with other levels. Typically this will only happen at points in  $g$ -space (although one can in principle have higher-dimensional singular "degeneracy hypersurfaces"). We thus have the typical (but not generic) situation shown in the picture,



where the field issues from "degeneracy sources", which can have either sign, and which have a strength defined by (52). To see better how this works one has to consider examples.

Thus we see that the Hamiltonian or " $g$ -space" conceals a hidden geometry, populated by the analogue of a static gauge field - indeed, there is a whole set of

these fields, one for each of the levels corresponding to state  $|n(g)\rangle$ . The whole structure is very complex, because the different levels are connected together by these degeneracies, and so one has the generalization to  $N$  dimensions (the dimension of  $g$ -space) of a set of Riemann sheets.

If the number of levels that becomes degenerate exceeds two and/or if the degeneracy persists over a region of  $g$ -space, then it is simpler to rediscuss the whole problem in terms of a manifold of states. Thus, suppose the adiabatic states take the form:

$$H(g) \phi_{n\nu}(g) = E_n(g) \phi_{n\nu}(g) \equiv E_n(g) |n\nu_n(g)\rangle \quad (53)$$

where  $\nu_n = 1, \dots, p_n$  label a set of  $p_n$  different degenerate states, making up the manifold  $\{\phi_{n\nu}(g)\}$  of these states in Hilbert space. The total wave function is then

$$\psi(t) = \sum_n \sum_{\nu_n} C_{n\nu_n}(t) e^{-\frac{i}{\hbar} \int dt' E_n(g(t'))} |n\nu_n(g(t))\rangle \quad (54)$$

and the coefficients  $C_{n\nu_n}(t)$  obey the eqn of motion

$$\left. \begin{aligned} \dot{C}_{m\alpha_m}(t) &= - \sum_n \sum_{\nu_n} \langle m\alpha_m | \partial_t | n\nu_n \rangle C_{n\nu_n}(t) e^{-\frac{i}{\hbar} \int dt' (E_n(g(t')) - E_m(g(t')))} \\ &\equiv i \sum_n \sum_{\nu_n} \underline{A}_{mn}^{\alpha_m \nu_n}(g(t)) \cdot \dot{g}(t) C_{n\nu_n}(t) e^{-\frac{i}{\hbar} \int dt' (E_n(g(t')) - E_m(g(t')))} \end{aligned} \right\} \quad (55)$$

$$\text{where} \quad \underline{A}_{mn}^{\alpha_m \nu_n}(g) = i \langle m\alpha_m | \nabla_g | n\nu_n \rangle \quad (56)$$

These eqns are the generalizations of (32), (33), (37), & (38). Now let us specialize to the  $n$ -manifold, assuming these states do not interact with (ie make transitions to) any other manifold. We then have, generalizing (39), that

$$\left. \begin{aligned} \dot{C}_{n\mu_n}(t) &= - \langle n\mu_n | \partial_t | n\nu_n \rangle C_{n\nu_n}(t) \\ &\equiv i \dot{g} \cdot \underline{A}_n^{\mu\nu}(g) C_{n\nu_n}(t) \end{aligned} \right\} \quad (57)$$

and the generalization of (43), the wave-function inside the  $n$ -manifold at time  $t$ , is

$$\psi_{n\mu}(t) = e^{i \underline{\Phi}_n^{\mu\nu}(t)} |n\nu(g(t))\rangle \quad (58)$$

where the Berry and dynamical phases are now matrix quantities:

$$\Phi_n^{M\nu}(t) = \phi_n^{M\nu}(t) + \gamma_n^{M\nu}(t) \quad (59)$$

with

$$\phi_n^{M\nu}(t) = \delta_{\mu\nu} \frac{1}{\hbar} \int dt' E_n(g(t')) \quad (60)$$

$$\left. \begin{aligned} \gamma_n^{M\nu}(t) &= \int_{g(0)}^{g(t)} \dot{g} \cdot \underline{A}_{nn}^{M\nu}(g(t')) \\ &\equiv \int_{g(0)}^{g(t)} dg \cdot \underline{A}_{nn}^{M\nu}(g) \end{aligned} \right\} \quad (61)$$

Thus we are dealing with a non-Abelian ( $SU(p_n)$ ) generalisation of the original Berry phase. The resulting field is more complicated: one has

$$\underline{D}_{nn}^{M\nu}(g) = \nabla_g \times \underline{A}_{nn}^{M\nu}(g) - i (\underline{A}_{nn}(g) \times \underline{A}_{nn}(g))^{M\nu} \quad (62)$$

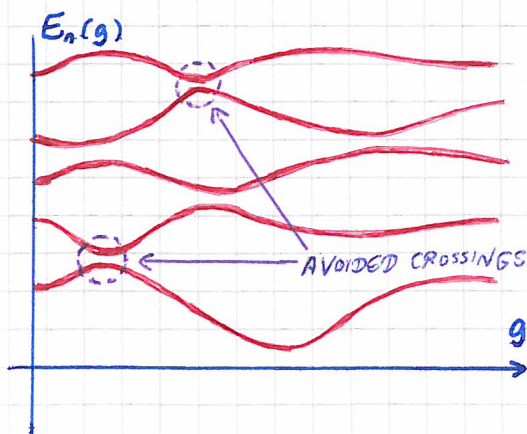
with a corresponding increase in complexity of the field configurations. I will not pursue this interesting topic further here.

## 1(c) TRANSITIONS IN THE ADIABATIC REGIME

None of the above discussion took account of transitions between the different levels as one varied  $g(t)$ ; it was assumed that these were negligible (and they must be in the adiabatic limit - this is the context of the Q. adiabatic theorem).

However it is not obvious from eqns. (34) or (55) what these transition amplitudes must be; nor is it even obvious that they go to zero in the adiabatic limit. A proper investigation of this question leads to some interesting mathematics, and a very useful formula, known as the "Landau-Dykhne" formula.

We consider the situation shown below, where the energy levels of some

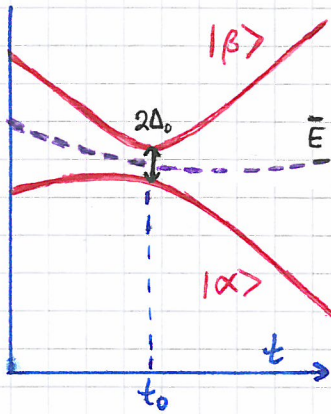


quantum system we plotted as a function of a single parameter  $g$ , a coupling in the Hamiltonian. Obviously we could imagine a set of hypersurfaces, which we the energy surfaces  $E_n(g)$ ; but we will not need these here, since we will only ever look at a particular path  $g(t)$  followed by the system over time  $t$ . Thus

We can think of  $g(t)$  as following this curve, and the plot on the previous page is just  $E_n(g(t))$  along this curve.

It is clear that as we change  $g(t)$  in time, the transitions will mostly occur at the "avoided crossings" shown in the picture. This is already clear from lowest-order time-dependent perturbation theory, (see, eg., eqns. (16) & (18)). However this gives no clear picture of the true structure of the problem, which is non-perturbative.

In what follows we consider the problem of transitions between a single pair of levels  $|\alpha\rangle$  and  $|\beta\rangle$ . This simplification, it turns out, captures most of the essential physics; moreover, the problem for a set of  $n > 2$  interacting levels is still not fully understood.



The situation is thus as shown at left. As  $t$  varies, a pair of levels  $|\alpha\rangle, |\beta\rangle$  vary in time - these are the adiabatic levels, defined by (cf. (32)):

$$H(g(t)) |\alpha(g)\rangle = E_\alpha(g) |\alpha(g)\rangle \tag{63}$$

and we assume that the complete wave-fn. as a function of time is (cf. (33)):

$$\psi(t) = \sum_{\alpha=1,2} C_\alpha(t) \phi_\alpha(g(t)) e^{-\frac{i}{\hbar} \int dt' E_\alpha(t')} \tag{64}$$

As the levels evolve in time, so does their mean energy  $\bar{E}(g(t))$  and their difference  $E(g(t))$ , given by

$$\left. \begin{aligned} \bar{E}(g) &= \frac{1}{2} (E_1(g) + E_2(g)) \\ E(g) &= \frac{1}{2} (E_2(g) - E_1(g)) \end{aligned} \right\} \tag{65}$$

At the distance of closest approach, we have  $E_{\min}(g) = \Delta_0$  (66)

corresponding to a minimum splitting of  $2\Delta_0$ .

(i) ADIABATIC EXPANSION = LOWEST-ORDER APPROXIMATION

If we compare the kind of expression that comes out of time-dependent pert. theory (cf., eg., (13), (14), & (16)), with the exact result for the time-dependent amplitudes in (34), it is clear that in the slow limit, we are expanding in the wrong parameter in expressions like (13) or (16). What we actually need to do is use the slowness of the changes in  $g(t)$  to expand in a dimensionless parameter like  $\epsilon$  in (41), or in  $1/t\epsilon_0$  in (40).

To do this, we return to the expression (34) for the time rate of change of the coefficients in  $\psi(t)$ , i.e. (PT0):

$$\dot{c}_\alpha(t) = - \langle \alpha | \partial_t \beta \rangle c_\beta(t) e^{-\frac{i}{\hbar} \int_{-\infty}^t (E_\beta(t') - E_\alpha(t')) dt'} \quad (67)$$

Here now we are only interested in the off-diagonal term. Now, even though we only consider 2 levels here, so that we simply have 2 coupled eqns for these 2 levels, nevertheless the problem is difficult to solve.

We notice that there is a small parameter in this problem, viz., the rate of transition  $\langle \beta | \partial_t \alpha \rangle$ ; this is small because, by hypothesis, we are working in the adiabatic regime. We can write a dimensionless expansion parameter

$$\begin{aligned} \gamma_{\alpha\beta}(t) &= \hbar \frac{\langle \alpha | \partial_t \beta \rangle}{E_\beta(t) - E_\alpha(t)} \equiv \frac{\langle \alpha | \partial_t \beta \rangle}{\omega_{\beta\alpha}(t)} \\ &\equiv -i \dot{g}(t) \frac{A_{\alpha\beta}(g(t))}{\omega_{\beta\alpha}(t)} \end{aligned} \quad (68)$$

or, alternatively, we can make the formal transformation

$$\Gamma_{\alpha\beta}^\lambda(t) = \langle \alpha | \partial_t \beta \rangle \rightarrow \lambda \Gamma_{\alpha\beta}^\lambda(t) = \lambda \langle \alpha | \partial_t \beta \rangle \quad (69)$$

and then treat the regime  $\lambda \ll 1$ , using  $\lambda$  as an expansion parameter. Using either of these manoeuvres, it is straightforward to derive an expansion for the transition amplitude.

Suppose we start the system in state  $|\alpha\rangle$ , so that

$$\psi(t = -\infty) = |\alpha\rangle \quad (70)$$

Then, to lowest order in  $\lambda$ , we have at time  $t$  the amplitude  $c_\beta(t)$  to find the system in the other state as

$$\begin{aligned} c_\beta(t) &= - \int_{-\infty}^t dt' \langle \beta | \partial_{t'} \alpha \rangle e^{-\frac{i}{\hbar} \int_{-\infty}^{t'} (E_\alpha(t'') - E_\beta(t'')) dt''} + O(\lambda^2) \\ &\equiv i \int_{-\infty}^t dt' \dot{g}(t') A_{\beta\alpha}(g(t')) e^{-i \int_{-\infty}^{t'} \omega_{\beta\alpha}(t'') dt''} + O(\lambda^2) \end{aligned} \quad (71)$$

Notice that we have seen this result before, in (16). Here, however, it appears as the first term in an infinite expansion—indeed, the final result can be written as a series of form

$$c_\beta(t) = c_\beta^{(1)}(t) + c_\beta^{(2)}(t) + \dots \quad (72)$$

$$\text{where } c_\beta^{(k+1)}(t) = - \int_{-\infty}^t dt' \langle \beta | \partial_{t'} \alpha \rangle c_\beta^{(k)}(t') e^{-i \int_{-\infty}^{t'} \omega_{\beta\alpha}(t'') dt''} \quad (73)$$

where we see that the  $k$ -th order term contains  $\langle \beta | \partial_t \alpha \rangle$  to the  $k$ -th power. (compare the structure of eqns (12), (22), (27)).

Equations like (73) can be evaluated using steepest descent methods. We do not pursue to do this here, since one actually finds that the transition amplitude is exponentially small in the parameter  $\hbar \omega_\beta$ , and that moreover so are the higher terms - they all contribute to the exponent, in general. Instead of studying this complicated topic here, we proceed to a rather different method of doing the calculation, which is actually exact, in the adiabatic limit.

(ii) LANDAU-DYKHNE FORMULA : As early as 1932, Landau had understood the importance & generality of the problems raised by the slow limit of QM (& also the related problems of tunneling & "suprabarrier reflection", and had developed a general method for handling them.

In this sub-section the basic result is explained, along with some remarks on the method. This method is rather subtle, and a proper understanding of it requires one to analyze the problem using the theory of asymptotic series - this will be done later.

As realized by Landau, the general problem is best approached by first looking at the 2-level problem described in eqns. (63)-(66). It is useful to write this in several forms. First, we write  $\mathcal{H}(g(t))$  in matrix form:

$$\mathcal{H}_{\text{op}}(g(t)) = \begin{pmatrix} H_{11}(t) & H_{12}(t) \\ H_{21}(t) & H_{22}(t) \end{pmatrix} = \bar{E}(t) + \begin{pmatrix} E(t) & \Delta(t) \\ \Delta(t) & -E(t) \end{pmatrix} \quad (74)$$

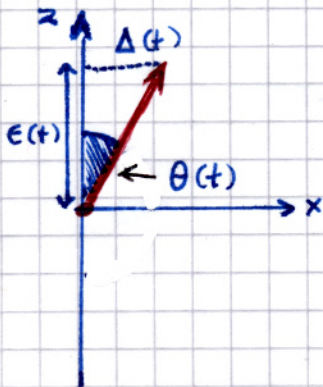
$$\text{so that the total splitting is } \left. \begin{aligned} 2E_0(t) &= 2(E^2(t) + \Delta^2(t))^{1/2} \\ \text{and} \quad E_{\pm}(t) &= \pm E_0(t) \end{aligned} \right\} \quad (75)$$

We can also write this in the trigonometric form

$$\mathcal{H}_{\text{op}}(t) = E_0(t) \begin{pmatrix} \cos \theta(t) & \sin \theta(t) \\ \sin \theta(t) & -\cos \theta(t) \end{pmatrix} \quad (76)$$

$$\text{where } \tan \theta(t) = \frac{\Delta(t)}{E(t)} \quad (77)$$

$$\text{ie } e^{2i\theta(t)} = \frac{E(t) - i\Delta(t)}{E(t) + i\Delta(t)}$$





The trigonometric picture shows how we can think of this system as a spin-1/2, in a  $t$ -dependent field of magnitude  $E_0(t)$ , in a direction in the  $zx$ -plane, with angle  $\theta(t)$ , measured from the  $z$  axis. If we allow a complex  $\Delta(t) = \Delta e^{i\phi}$ , then the field rotates into the  $xy$ -plane, with an angle  $\phi(t)$ . Here, to keep things simple, we assume that  $\Delta(t)$  is real.

We also can write the instantaneous quasi-static eigenfunctions for the system, as

$$|\phi_{\uparrow}(t)\rangle = \begin{pmatrix} \cos \theta/2 \\ -\sin \theta/2 \end{pmatrix} \quad |\phi_{\downarrow}(t)\rangle = \begin{pmatrix} \sin \theta/2 \\ \cos \theta/2 \end{pmatrix} \quad (78)$$

and this allows us to write the time-dependent level coupling in the simple form

$$\Gamma_{\uparrow\downarrow}(t) = \Gamma(t) = \langle \phi_{\uparrow} | \partial_t \phi_{\downarrow} \rangle = \frac{1}{2} \dot{\theta}(t) \quad (79)$$

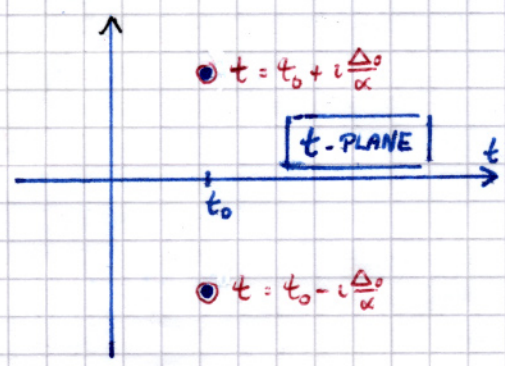
We begin by stating the Landau-Dykhne result, and then giving a somewhat heuristic argument to justify it. The result is as follows. We consider the Hamiltonian  $\mathcal{H}_{\text{top}}(t)$  now as a function of COMPLEX TIME  $\tau$ , and in general this means that the Hamiltonian itself will be complex. In general the Hamiltonian and its energy levels can be treated as complex variables, functions of complex  $t$ , with in the present case a level-crossing or crossings occurring in the complex plane. For the form as written in (74) this clearly happens when

$$E(\tau) = \pm i\Delta(\tau) \quad \Rightarrow \quad E_0(\tau) = 0 \quad (80)$$

and we see that the generic behaviour of the behaviour of  $E_0(\tau)$  in the complex plane, about a root of  $E_0$ , is

$$E(\tau) \xrightarrow{\tau \rightarrow \tau_0} C \sqrt{\tau - \tau_0} \quad (81)$$

where  $\tau_0$  is a root of the eqn (80), and  $C$  is a constant.



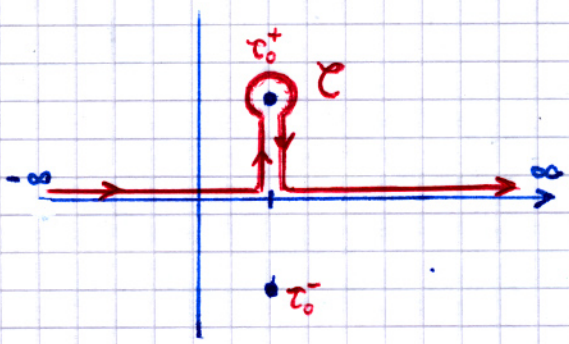
As an example of this, consider the famous Landau-Zener problem, for which

$$\Delta(t) = \Delta_0 \quad \epsilon(t) = \alpha(t - t_0) \quad (82)$$

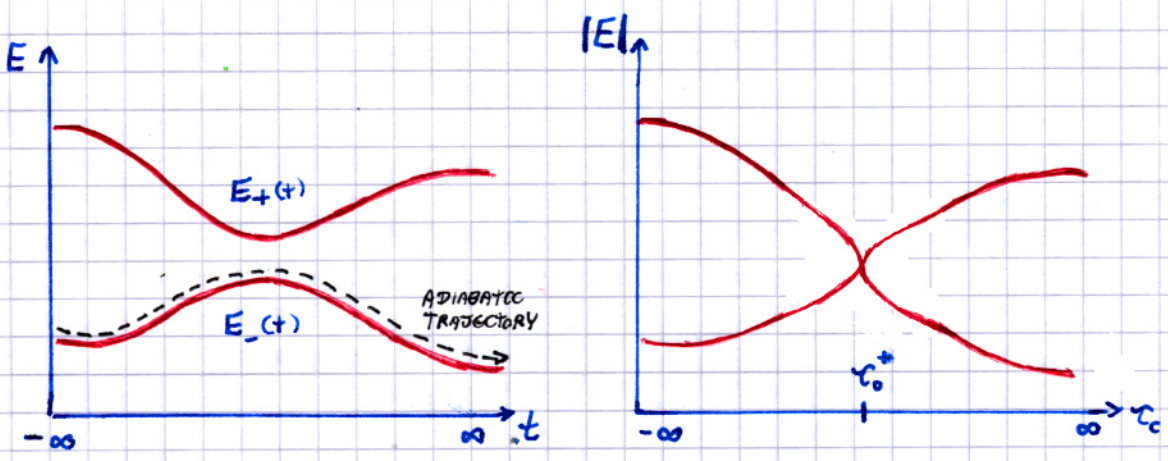
$$\text{so that } \tau_0^{\pm} = t_0 \pm i \frac{\Delta_0}{\alpha} \quad (83)$$

From this it immediately follows that the function  $E_0(\tau)$  must have one or more branch cuts in the  $\tau$ -plane, with the  $\tau_0^\pm$  constituting a pair of branch points.

Consider now the behaviour of the eigenfunctions (quasi-static) of the complex Hamiltonian  $\mathcal{H}(\tau)$ . This in general is quite a complicated job. However we notice that they will change rather rapidly in the vicinity of the points  $\tau_0$ , simply because we have a level-crossing there. To get an idea of what is going on, consider the problem where there is a single avoided crossing near  $t = t_0$ , and we wish to calculate the final state wave-function, given that the initial-state wave-fn is entirely in one of the 2 states.



Consider now the contour  $\mathcal{C}$  shown, in the  $\tau$ -plane, for this system. There is nothing to stop us analytically continuing the trajectory into the complex time domain, provided we cross no singularities (branch points or branch cuts). Now consider what will happen to the system under those circumstances.



In the left-hand graph we see the 2 energy levels of the quasi-static Hamiltonian in real time. These are entirely real, and there is an avoided level-crossing. Now, suppose we traverse the level-crossing regime, in this left-hand figure, extremely slowly. Then the quantum adiabatic theorem applies, and we must stay in the quasi-static state - the system follows the adiabatic trajectory shown in the figure.

Now examine the quasi-static states along the contour  $\mathcal{C}$ , shown in the right-hand figure. In this case there is no avoided crossings - the 2 levels become degenerate at the point  $\tau_0^+$  in the complex time regime (with the energies approaching each other like  $\sqrt{t - t_0^+}$ ).