

LECTURE 2

§3. DYNAMICS

So far we have not said anything about how ψ or ρ depends on time; and this is in many ways our central problem. There are, roughly speaking, 2 ways of doing this - the differential and the integral formulation. It is also useful to recall the formulation in the classical limit.

§3(a) CLASSICAL LIMIT

Recall that in the classical limit, the dynamics can be formulated as either a set of M differential eqns., for M degrees of freedom, in terms of the Lagrangian $L(\underline{Q}, \dot{\underline{Q}}; t)$:

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{Q}_j} \right) - \frac{\partial L}{\partial Q_j} = 0 \quad (3.1)$$

or a set of $2M$ differential eqns. in terms of the Hamiltonian:

$$\dot{Q}_j = \frac{\partial \mathcal{H}}{\partial P_j} \quad \dot{P}_j = - \frac{\partial \mathcal{H}}{\partial Q_j} \quad (3.2)$$

where

$$\mathcal{H}(\underline{P}, \underline{Q}; t) = \sum_j P_j \dot{Q}_j - L(\underline{Q}, \dot{\underline{Q}}; t) \quad (3.3)$$

The importance of this formulation is that we can in many cases find the quantum description from a known classical description by "quantizing"; and because \mathcal{H} and L obey variational equations which appear to be fundamental to all quantum theories so far discovered. The Lagrangian is related to the total action by

$$S = \int_{t_i}^{t_f} dt L(\underline{Q}, \dot{\underline{Q}}; t) \quad \left| \begin{array}{l} Q(t_f) = Q_f \\ Q(t_i) = Q_i \end{array} \right. \quad (3.4)$$

and Lagrange's eqns are derived by variation of S written in this form; the principle of least action states that

$$\delta S = \delta \int_{t_i}^{t_f} dt \left(\frac{\partial L}{\partial \underline{Q}} \cdot \delta \underline{Q} + \frac{\partial L}{\partial \dot{\underline{Q}}} \cdot \delta \dot{\underline{Q}} \right) \Big|_{\substack{\delta Q(t_f) = 0 \\ \delta Q(t_i) = 0}} = 0 \quad (3.5)$$

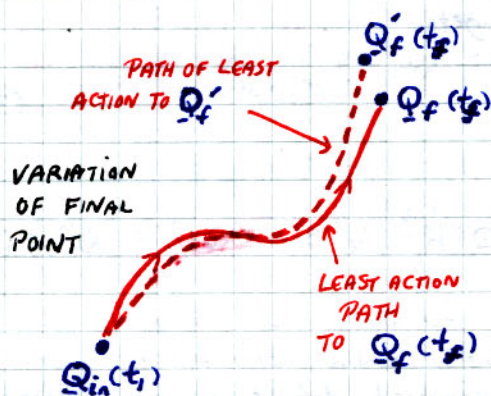
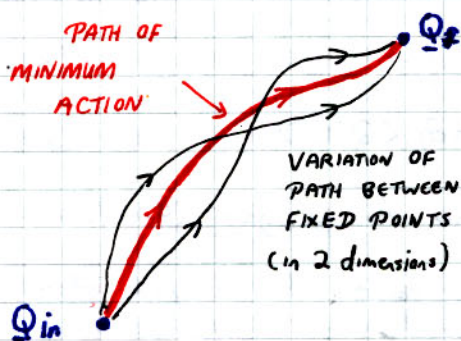
which leads immediately to (3.1). In classical mechanics this usually leads to a unique path, the extremal path for this action functional.

One can also derive Hamiltonians from a slightly different formulation of the

action principle. Instead of varying over all paths for which the end-points are fixed, one can consider varying paths by varying one of the end-points (but keeping t_2 and t_1 fixed).

In this case the variation instead becomes, instead of (3.5), the expression

$$\begin{aligned} \delta S &= \delta \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial \dot{Q}} \cdot \delta \dot{Q} + \frac{\partial L}{\partial Q} \cdot \delta Q \right) \\ &= \left[\frac{\partial L}{\partial \dot{Q}} \cdot \delta Q \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} dt \left(-\frac{d}{dt} \frac{\partial L}{\partial \dot{Q}} + \frac{\partial L}{\partial Q} \right) \cdot \delta Q \\ &= 0 \end{aligned} \quad (3.6)$$



but now the first term (the integrated term) is no longer zero. Suppose we let $\delta Q(t_1) = 0$, and only allow $\delta Q(t_2)$ to be finite. Then, since (3.1) is still true, and writing

$$\underline{P} = \partial L / \partial \dot{Q} \quad (3.7)$$

we have

$$\delta S = \underline{P} \cdot \delta Q \quad (3.8)$$

which is the same as saying that

$$\partial S / \partial Q_j = P_j \quad (3.9)$$

Finally, we can also vary t_2 ; this gives

$$\partial S / \partial t = L - \underline{P} \cdot \dot{Q} \quad (3.10)$$

or, in differential form, and using (3.3),

$$\frac{\partial S}{\partial t} + H(\underline{P}, \underline{Q}; t) = 0 \quad (3.11)$$

which is the Hamilton-Jacobi eqn.

All of these formulations have interesting relationships to the quantum formalism, which will appear several times as we go along. Most important is the "flow" of trajectories in either $(\underline{Q}, \dot{\underline{Q}})$ space or in $(\underline{P}, \underline{Q})$ space. The flow in phase space, which is best understood starting from a Hamiltonian formulation of the least action principle, is

$$\delta S = \delta \int P_j dQ_j - H dt \quad (3.12)$$

is particularly useful when one comes to classical statistical mechanics, in which one deals with a probability function in phase space - we will return to this below. Note that (3.12) is derived by varying δt_f .

Exercise: Work out all of the above for the specific case of a rotating rigid body, with angular momentum/angle as coordinates.

3(b) QUANTUM MECHANICS - DIFFERENTIAL EQTN. FORM

This is so well known that I simply remind you of the results. The Schrödinger eqn. is, for any non-relativistic system:

$$\hat{H}_0 \psi = i\hbar \partial_t \psi \quad (3.13)$$

$$\text{ie } \langle Q | \hat{H}_0 | Q_0 \rangle \langle Q_0 | \psi \rangle = i\hbar \partial_t \langle Q | \psi \rangle. \quad (3.14)$$

The first eqn defines a "flow" in Hilbert space for a given Hamiltonian - we shall say a little more about this later.

The density matrix also obeys a differential equation. For a pure state, in which $\rho(Q, Q') = \langle Q | \psi \rangle \langle \psi | Q' \rangle$, this eqn is trivial to derive from (3.13) or (3.14), and one gets

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] \quad (3.15)$$

ie.,

$$\partial_t \langle Q | \hat{\rho} | Q' \rangle = -\frac{i}{\hbar} (\langle Q | \hat{H}_0 \rho | Q' \rangle - \langle Q | \hat{\rho} \hat{H}_0 | Q' \rangle) \quad (3.16)$$

However, it is easily seen that this formula is also true for an arbitrary mixture or for a reduced density matrix, because it holds for each "component" of these (with component defined in the diagonal representation, ie., that part having probability p_j - cf. (1.2)); we can thus write the proof in the diagonal representation, and any subsequent unitary transformation does not change this. Notice that this also means that the different components are not "mixing" in time - this is physically obvious. As a corollary we have that, for a pure state (for which we use the subscript "0"):

$$\left. \begin{aligned} \rho_0^2(t) &= \rho_0(t) && \text{(PURE STATE)} \\ \text{(if } \rho_0^2(t=t_n) &= \rho_0(t=t_n)) \end{aligned} \right\} \quad (3.17)$$

ie., a pure state cannot evolve into a mixture (unless the Hamiltonian changes, of course! Obviously if we switch on a coupling to some other system, this allows such an evolution).

A warning - do not confuse (3.15) with an eqn. for an operator written in the Heisenberg representation. Unless stated otherwise, we will stay in the Schrödinger representation.

3(c) QUANTUM MECHANICS - INTEGRAL FORM

By an integral form for Q.M. we can mean either (i) the solution for $\psi(x,t)$ written in terms of an integral, or (ii) the Schrödinger eqn written as an integral eqn. No theory or derivations will be developed here - this can all be found in the books and in the usual courses.

Perhaps the most obvious way to set up an integral description of the wave-fn. evolution is by direct integration of (3.13). This is simple if the Hamiltonian is time-INDEPENDENT; then we have

$$\psi(t) = e^{-\frac{i}{\hbar} \hat{H}_0(t-t_0)} \psi(t_0) \equiv \hat{U}_0(t-t_0) \psi(t_0) \quad (3.18)$$

and this eqn is then most easily projected onto the eigenstates of \hat{H} , i.e.,

$$\text{if } \hat{H}_0 \psi_n = E_n \psi_n \quad \psi_n(t) = e^{-\frac{i}{\hbar} E_n(t-t_0)} \psi_n(t_0) \quad (3.19)$$

However in any other representation, involving a complete set of states like the $\{|\varphi\rangle\}$, we must take account of the operator nature of \hat{H} . Let us do this in a very simple way; from (3.18) we can write (letting $|\psi_m(t)\rangle = |m(t)\rangle$):

$$\begin{aligned} \langle \varphi | \psi(t) \rangle &= \langle \varphi | e^{-\frac{i}{\hbar} \hat{H}_0(t-t_0)} | \psi(t_0) \rangle \\ \text{i.e.} \quad &= \langle \varphi | m \rangle \langle m | e^{-\frac{i}{\hbar} \hat{H}_0(t-t_0)} | m \rangle \langle m | \varphi_0 \rangle \langle \varphi_0 | \psi(t_0) \rangle \\ &= \sum_m \psi_m(\varphi) \psi_m^*(\varphi_0) e^{-\frac{i}{\hbar} E_m(t-t_0)} \langle \varphi_0 | \psi(t_0) \rangle \end{aligned} \quad (3.20)$$

$$\text{which we write as } \psi(\varphi, t) = \int G_0(\varphi, \varphi_0; t, t_0) \psi(\varphi_0, t_0) d\varphi_0 \quad (3.21)$$

where

$$G_0(\varphi, \varphi_0; t, t_0) = \sum_m \psi_m(\varphi) \psi_m^*(\varphi_0) e^{-\frac{i}{\hbar} E_m(t-t_0)} \quad (3.22)$$

More generally we define this Green function or "propagator" by the differential eqn:

$$\left. \begin{aligned} (\hat{H}_0 - i\hbar \partial_t) G_0(\varphi, \varphi_0; t, t_0) &= -i\hbar \delta(\varphi - \varphi_0) \delta(t - t_0) \\ \text{or } (\hat{H}_0 - i\hbar \partial_t) \langle \varphi | \hat{G}_0(t, t_0) | \varphi_0 \rangle &= -i\hbar \delta(t - t_0) \langle \varphi | \hat{1} | \varphi_0 \rangle \end{aligned} \right\} \quad (3.23)$$

where in the second eqn we introduce the operator $\hat{G}_0(t, t_0)$, which by comparing with (3.20) is obviously also writeable as

$$\hat{G}_0(t, t_0) = \sum_m |m\rangle e^{-\frac{i}{\hbar} E_m(t-t_0)} \langle m| \quad (3.24)$$

Exercise: Prove that the functions G_0 in (3.23) and (3.22) are the same functions.

Another useful way of writing the Green function is to Fourier transform to the frequency domain - notice that if \hat{H} is time-independent, then $G_0(t, t_0)$ must be a function only of $(t-t_0)$ (the system is invariant under any

displacement in the time domain). Thus we write

$$\begin{aligned}\hat{G}_0(\omega) &= \int_{-\infty}^{\infty} dt \hat{G}_0(t) e^{i\omega t} \\ &= \int_{-\infty}^{\infty} dt e^{i(\omega - \hat{H}/\hbar)t}\end{aligned}\quad (3.25)$$

which gives

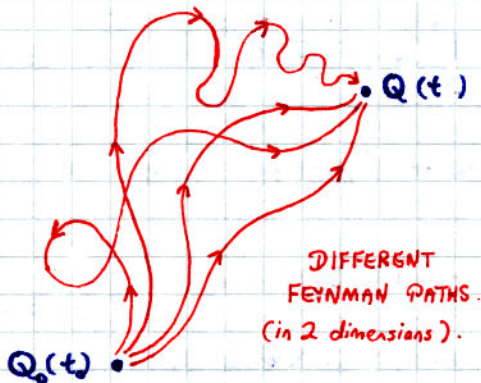
$$\hat{G}_0(\omega) = \frac{i}{\omega - \hat{H}/\hbar} \quad (3.26)$$

$$G_0(\varphi, \varphi_0; \omega) = \sum_m \frac{\psi_m^+(\varphi) \psi_m(\varphi_0)}{\omega - \epsilon_m/\hbar} \quad (3.27)$$

I won't go into the various analytic properties of $G(\omega)$ in the complex ω -plane.

Now, it was discovered by Feynman that there is another very nice way to write the propagator, as a functional integral summing over all possible intermediate states, or "paths", between the states $\psi(\varphi_0, t_0)$ and $\psi(\varphi, t)$, in (3.21). This is known as the PATH INTEGRAL formalism. The remarkable result is that we can also write

$$G_0(Q, Q_0; t, t_0) = \int_{q(t_0)=Q_0}^{q(t)=Q} \mathcal{D}q(\tau) e^{i/\hbar S_0[q, \dot{q}]} \quad (3.28)$$



The meaning of this expression is that we sum over all paths $q(\tau)$, as a function of time τ , which start at $Q_0(t_0)$ and finish at $Q(t)$. Associated with each path is the factor

$$\begin{aligned}e^{i/\hbar S_0[q, \dot{q}]} &= e^{i/\hbar \int_{t_0}^t dt L_0(q(\tau), \dot{q}(\tau))} \\ &= e^{i\varphi_0[q, \dot{q}]}\end{aligned}\quad (3.29)$$

so that when we sum over all paths, extensive phase interference takes place between the paths - the problem ends up looking like an optics problem.

The mathematical problem of properly defining this integral for "all paths" is non-trivial (what measure is assigned to different paths? How "crooked" can they be? etc.); I won't discuss this here, since you can learn it in the usual courses or texts.

Note that there is nothing to force us to choose the real space paths for this problem, except that it is convenient to do so if the Lagrangian is written in terms of real space velocities and coordinates. However these coordinates may be quite irrelevant for some problems (eg., for angular momenta or spins - in the latter case there is no classical Lagrangian!),

and so one obviously has to deal with other kinds of path. In fact we have already looked at other paths, in the brief treatment of the central spin model given in §2; we return to this below.

Note also that, just as in the classical case, we do not have to define the action in terms of the Lagrangian. Thus, instead of (3.28) we can also write the Green function in the form

$$G_0(Q, Q_0; t, t_0) = \int_{q(t_0)=Q_0}^{q(t)=Q} \mathcal{D}q \mathcal{D}p e^{i/\hbar S_0[q, p]} \quad (3.30)$$

$$S_0[q, p] = \int_{t_0}^t dt (P\dot{Q} - \mathcal{H}_0(P, Q)) \quad (3.31)$$

and such "phase space" path integrals can sometimes be useful (although it turns out that the problem of the measure of paths in phase space is really acute, and (3.30) can actually give nonsense results under some circumstances).

Consider now the density matrix. For a pure state the generalisation of (3.21) and (3.22) is fairly obvious; we have

$$\rho_0(Q, Q'; t) = \int dQ_0 dQ'_0 K_0(Q, Q'; Q_0, Q'_0; t, t_0) \rho_0(Q_0, Q'_0; t_0) \quad (3.32)$$

with

$$K_0(Q, Q'; Q_0, Q'_0; t) = \sum_{m, n} \psi_m(Q) \psi_m^*(Q_0) \psi_n(Q') \psi_n^*(Q'_0) \times e^{-i/\hbar E_m(t-t_0)} e^{i/\hbar E_n(t-t_0)} \quad (3.33)$$

i.e., that the propagator for the pure state density matrix can be written as

$$\left. \begin{aligned} K_0(Q, Q'; Q_0, Q'_0; t) &= \langle Q, Q'_0 | \hat{K}_0(t, t_0) | Q_0, Q' \rangle \\ \hat{K}_0(t, t_0) &= \sum_{m, n} |mn\rangle e^{-i/\hbar [E_m - E_n](t-t_0)} \langle mn| \end{aligned} \right\} \quad (3.34)$$

where $|QQ'\rangle \equiv |Q\rangle|Q'\rangle$, and $|mn\rangle \equiv |m\rangle|n\rangle$, etc. In the same way we have

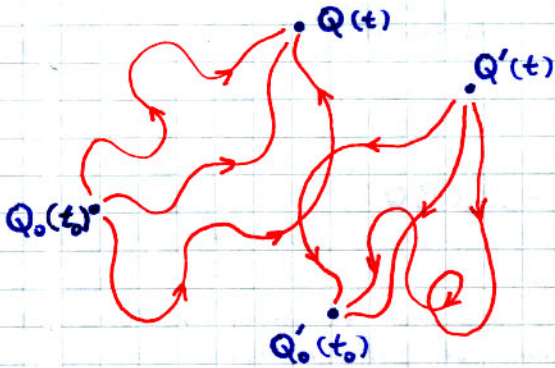
$$\begin{aligned} (\hat{H}_0 - i\hbar\partial_t) K_0(Q, Q'; Q_0, Q'_0; t-t_0) &= (\hat{H}_0 - i\hbar\partial_t) \langle QQ'_0 | \hat{K}_0(t-t_0) | Q_0, Q' \rangle \\ &= -i\hbar \langle QQ'_0 | \mathbb{1} | Q_0, Q' \rangle \delta(t-t_0) \\ &= -i\hbar \delta(Q-Q_0) \delta(Q'-Q'_0) \delta(t-t_0) \end{aligned} \quad (3.35)$$

for the differential eqn. governing K (which is also a Green function, but now for

the time evolution of P_0 .

For these "free" Green functions G_0 and K_0 the dynamics is that of a single isolated quantum system. This is also seen in the path integral expression for K_0 , which is an obvious generalisation of (3.28); we have

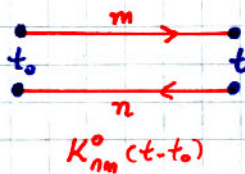
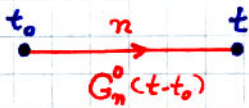
$$K_0(Q, Q'; Q_0, Q'_0; t-t_0) = \int_{\substack{q(t)=Q \\ q(t_0)=Q_0}} \mathcal{D}q(\tau) \int_{\substack{q'(t)=Q' \\ q'(t_0)=Q'_0}} \mathcal{D}q'(\tau) e^{-\frac{i}{\hbar} \{S_0[q, \dot{q}] - S_0[q', \dot{q}']\}} \quad (3.36)$$



where the paths are now between the states $|Q_0, Q'_0\rangle$ and $|Q, Q'\rangle$. In the drawing the arrow directions do not denote the direction of time τ in the usual way, but instead they denote the sense of evolution of the relevant phase in the expression - because $|\psi\rangle$ is paired with $\langle Q, Q'_0|$, whilst $\langle \psi|$ is paired with $|Q', Q_0\rangle$.

As noted above, there is nothing that forces us to project the propagators onto real space Hilbert states like $|Q\rangle$ or $|Q'\rangle$. By far the simplest projection is onto the eigenstates of \hat{H}_0 , i.e., we look at

$$\begin{aligned} \langle n | \hat{G}_0 | n' \rangle &= \sum_m \langle n | m \rangle e^{-\frac{i}{\hbar} \epsilon_n (t-t_0)} \langle m | n' \rangle \\ &= e^{-\frac{i}{\hbar} \epsilon_n (t-t_0)} \delta_{nn'} \end{aligned} \quad (3.37)$$



which is necessarily diagonal in $|n\rangle$ -space; the same can obviously also be done for the density matrix propagator:

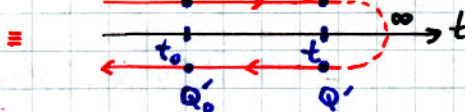
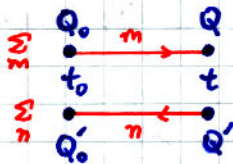
$$\langle n, m | \hat{K}_0(t-t_0) | n', m' \rangle = e^{-\frac{i}{\hbar} (\epsilon_m - \epsilon_n) (t-t_0)} \delta_{nn'} \delta_{mm'} \quad (3.38)$$

with the arrows again indicating the direction of phase evolution, as defined by the sense of the frequency oscillations (dynamic phase).

$$\sum_m \begin{array}{c} \xrightarrow{m} \\ Q_0(t_0) \quad Q(t) \end{array} \equiv \sum_m \langle Q_0 | m \rangle \xrightarrow{m} \langle m | Q \rangle \quad (3.39)$$

$$\equiv G_0(Q, Q_0; t-t_0)$$

Here we show 2 other ways of plotting these propagators.



$$\equiv K_0(Q, Q_0; Q', Q'_0; t-t_0)$$

$$(3.40)$$

Note that the way of plotting K_0 along a single path involves coming back in the reverse direction. Do NOT connect this with Feynman's propagation of holes back in time (which is something quite different). It is in fact more

useful to connect it with the Keldysh/Mills diagram technique for non-equilibrium systems (which we will come to).

3(d) REDUCED DENSITY MATRIX

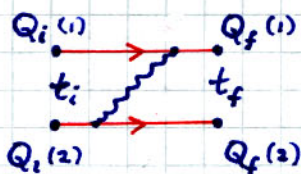
Up till now we have only looked at the density matrix/wave-function evolution for an isolated system. But what is much more interesting is the time evolution of either a mixed state, or of a "reduced" density matrix.

Note at this point something that is already demonstrated by what was said in §1, but which needs emphasis. There is no way ~~to~~ to tell the difference between a mixed state $\hat{\rho}_{\text{mixed}}(t)$ and a reduced density matrix $\bar{\rho}(t)$, for a given system - this follows from the discussion in section §1(a). Thus there should be no formal difference in the description of their dynamics - any time evolution of a $\hat{\rho}_{\text{mixed}}(t)$ can be simulated by ~~the~~ averaging over some external system which is coupled to it, and vice-versa (although this may involve some rather strange Hamiltonians, with interesting explicit time-dependence!).

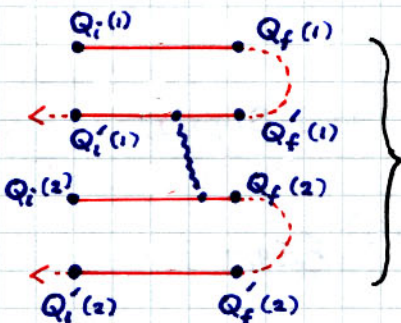
Let's get a first look at how this works, by considering a general Hamiltonian of form:

$$H(1,2) = H_0(1) + H_{\text{int}}(1,2) + H_{\text{ext}}(2) \quad (3.41)$$

i.e., a Hamiltonian of the type exemplified in section 2(c); we consider the 2nd system to be "external", and we will average it. First note that if we do NOT average over it, we have a rather horrible propagator for the pair of systems:



$$G_{12}(Q_f(1)Q_f(2); Q_i(1)Q_i(2); t_f - t_i) = \int \mathcal{D}q_1 \int \mathcal{D}q_2(\tau) e^{-\frac{i}{\hbar} S[q_1, q_2, \dot{q}_2]} \quad (3.43)$$



$$K_{12}(Q_f(1)Q_f'(1); Q_f(2)Q_f'(2) | Q_i(1)Q_i'(1)Q_i(2)Q_i'(2)) = \int_i^f \mathcal{D}q_1 \mathcal{D}q_2 \int_i^f \mathcal{D}q_1' \mathcal{D}q_2'(\tau) \times e^{-\frac{i}{\hbar} \{ S[q_1, q_2, \dot{q}_2] - S[q_1', q_2', \dot{q}_2'] \}} \quad (3.44)$$

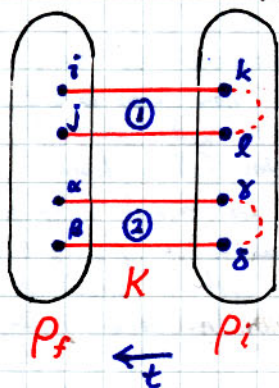
where I don't bother to put in all the limits in the path integrals - they are obvious from the diagram. Note immediately a crucial difference here - the 2 systems can interact (a single interaction is shown in the diagrams). The expressions of course simplify if $H_{\text{int}}(1,2) = 0$, because then we can simply

add the actions; $S(1,2) = S_0(1) + S_{ext}(2)$. But now we have

$$S(1,2) = S[q_1, \dot{q}_1, q_2, \dot{q}_2] = S_0[q_1, \dot{q}_1] + S_{ext}[q_2, \dot{q}_2] + S_{int}[q_1, \dot{q}_1, q_2, \dot{q}_2] \quad (3.45)$$

Now, suppose we average over system 2; how is this implemented formally? We have such a formal mess here that it is convenient to go back to the notation in §1 (eqns. (1.13) - (1.17)). Then for the eqn of motion of the pair of systems, we just have

$$P_{\gamma\mu\beta}^f(1,2;t_f) = \sum_{kl} \sum_{\gamma\delta} K_{\gamma\mu\beta;kl\gamma\delta}^{fi}(1,2;t_f,t_i) \rho_{kl\gamma\delta}^i(1,2;t_i) \quad (3.46)$$



or, even more concisely

$$P_{\gamma\mu\beta}^f = K_{\gamma\mu\beta;kl\gamma\delta} P_{kl\gamma\delta}^i \quad (3.47)$$

Now, if the final state is described by a reduced density matrix, we must clearly Trace over all final states of system 2. But this doesn't necessarily mean we want to trace over the initial state. For example,

a situation can arise in which we "prepare" both system 1 and system 2 together, in some way or another - and then let things evolve, with the interactions between 1 and 2 causing dynamic entanglement between them. In this case there would be no trace over the initial ρ^i , but the final density matrix would trace over all "unobserved" variables (ie, over the variables of system 2, if we only look at system 1). Thus there is a wide range of possibilities which we can define. For the moment let's just consider the simplest, where the initial GLOBAL density matrix $\rho_{kl\gamma\delta}^i$ is given, but we trace over the final states of 2. Then

$$\begin{aligned} \bar{\rho}_{ij}^f &= \text{Tr}_\alpha \rho_{ij\alpha\alpha}^f \\ &= \sum_\alpha K_{ij\alpha\alpha;kl\gamma\delta} P_{kl\gamma\delta}^i \end{aligned} \quad (3.48)$$

$$\equiv \bar{K}_{ij;kl\gamma\delta} P_{kl\gamma\delta}^i \quad (3.49)$$

where

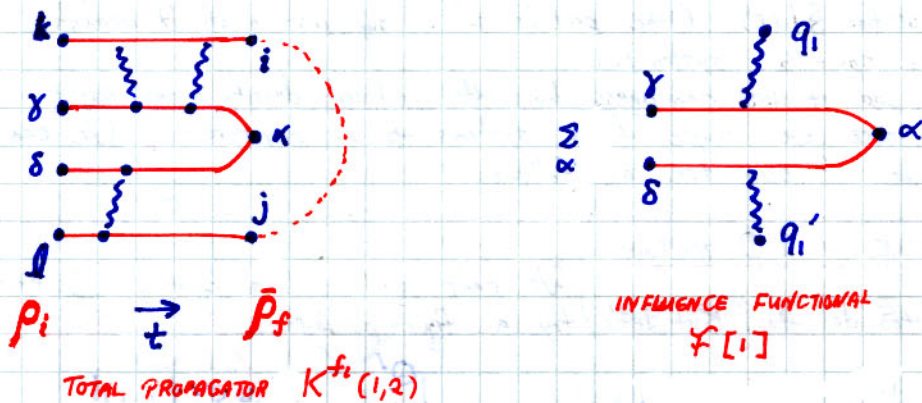
$$\bar{K}_{ij;kl\gamma\delta} = \sum_\alpha \int_{kl}^{ij} \mathcal{D}q_1 \mathcal{D}q_1' \int_{\gamma\delta}^{\alpha\alpha} \mathcal{D}q_2 \mathcal{D}q_2' e^{-\frac{i}{\hbar}(S[q_1, q_2] - S[q_1', q_2'])} \quad (3.50)$$

$$\equiv \int_{kl}^{ij} \mathcal{D}q_1 \mathcal{D}q_1' e^{-\frac{i}{\hbar}(S_0[q_1] - S_0[q_1'])} \mathcal{F}_{\gamma\delta}^f[q_1, q_1'] \quad (3.51)$$

where

$$\mathcal{F}_{\gamma\delta}^f[q_1, q_1'] = \sum_\alpha \int_{\gamma\delta}^{\alpha\alpha} \mathcal{D}q_2 \mathcal{D}q_2' e^{-\frac{i}{\hbar}(S_{int}[q_1, q_2] - S_{int}[q_1', q_2'] + S_{ext}[q_2] - S_{ext}[q_2'])} \quad (3.52)$$

where the functional or "kernel" $\mathcal{F}[q, q']$ is the "influence functional", invented by Feynman and Vernon (and essentially in previous work by Feynman & collaborators). We can give (3.49)-(3.52) a diagrammatic interpretation:



The influence functional is a "weighting" functional over different paths $(q_i(\tau), q_i'(\tau))$ of the control system 1, the one we are interested in.

We notice that if the system 2 doesn't interact with system 1, then clearly

$$\mathcal{F}[q, q'] \xrightarrow{\text{no interaction}} 1 \quad (3.53)$$

because then the system must evolve according to K_0 in (3.34). How does $\mathcal{F}[q, q']$ weight the paths? Well, in general, it must have the form

$$\mathcal{F}[q, q'] = e^{-i/\hbar (\Phi[q, q'] - i\Gamma[q, q'])} \quad (3.54)$$

where $\Phi[q, q']$ is a generalised phase functional, measuring the reactive or "renormalising" influence of the system 2 on system 1, and $\Gamma[q, q']$ is a decoherence functional, measuring the real suppression of matrix elements between q_i and q_i' in $\bar{\rho}(q_i, q_i')$, as time passes.

There is another way to write $\mathcal{F}[q, q']$ which is also very instructive. We note that it also describes the evolution of the external system 2 in the presence of a coupling to system 1, under the assumption that system 1 follows a certain path - and then one traces over system 2. Thus we can also write

$$\mathcal{F}[q, q'] = \langle \hat{U}_2[q_i(\tau)] \hat{U}_2^\dagger[q_i'(\tau)] \rangle \quad (3.55)$$

where $\hat{U}_2[q_i(\tau)]$ is the unitary operator describing the evolution of system 2 under the influence of an interaction with system 1, when system 1 travels along the path $q_i(\tau)$. The brackets $\langle \dots \rangle$ indicate the trace over the variables of system 2 - again, how we do this trace depends on our assumptions. Thus, the trace in (3.52) is an average

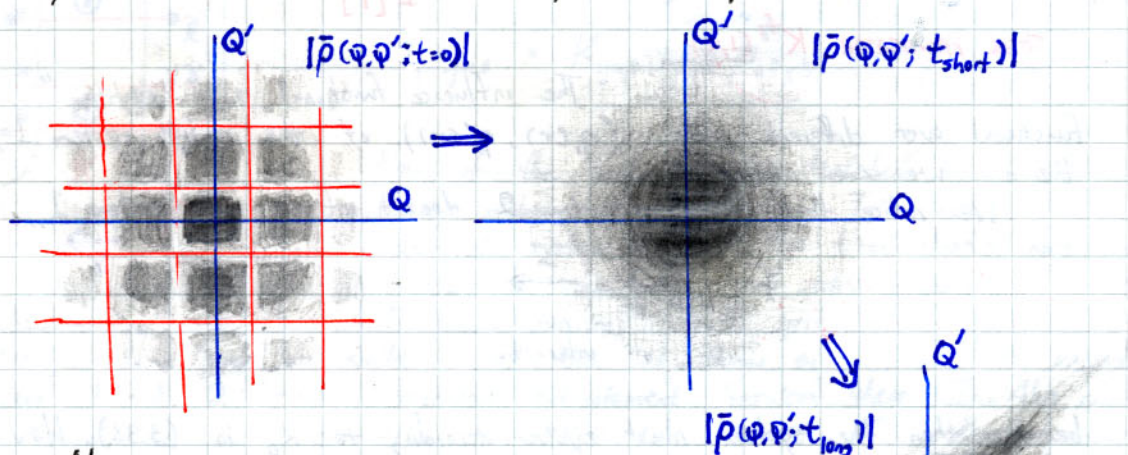
over final states of 2, but not over initial states.

From (3.54) we see that the interaction with the environment (system 2) can play havoc with the time evolution of the density matrix of system 1. It is interesting to think about this pictorially. Consider the 2 examples discussed in section §1(c) (the particle in a superposition of 2 momentum states, and the $spn = 1/2$ system).

Let us see if we can guess how the reduced density matrix might evolve in time, once we couple these systems to an environment. We can imagine a number of possibilities, as follows:

(a) PARTICLE IN 1-D MOTION

We can't yet calculate anything - I haven't told you how to do this. But let's try a few possibilities:



Here we imagine a situation in which the interference between the 2 momenta is quickly destroyed, followed by a slower destruction all off-diagonal matrix elements - so that finally we get something like a classical mixture, described by a probability function

$$\bar{\rho}(Q) = \bar{\rho}(Q, Q). \quad (3.56)$$

Does this happen? It depends of course on the nature of the environment, how it evolves in time, and what are the couplings to the particle. All of this is described by the influence functionals.

(b) TWO-LEVEL SYSTEM

Here it is simpler to just plot the behaviour of the density matrix elements as a function of time. There are 2 interesting limits, viz., when the bias ξ is zero (so that $|1\rangle$ and $|2\rangle$ are degenerate), and the case of strong bias, when $\xi \gg \Delta$ (i.e., $|1\rangle$ and $|2\rangle$ are way off resonance).

Before looking at the effect of the environment, let's just look at the behaviour of the 2-level system in its absence. This is trivial to calculate, directly from (3.18) and/or (3.34). Our Hamiltonian is,

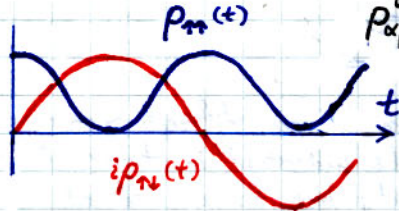
in the usual basis of $|\uparrow\rangle, |\downarrow\rangle$ states (cf. (2.1) or (2.12)):

$$\hat{H}_0 = \Delta \hat{c}_x + \xi_0 \hat{c}_z \quad \Rightarrow \quad \begin{pmatrix} \xi_0 & \Delta \\ \Delta & -\xi_0 \end{pmatrix} = \mathcal{H}_{\text{eff}}^0 \quad (3.57)$$

and the time-dependence of the matrix elements of $\hat{\rho}$ are then easily found:

(i) $\xi_0 = 0$

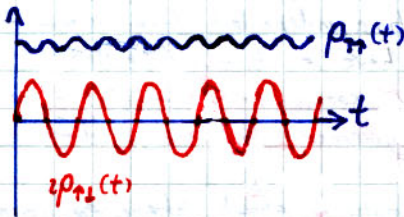
$$\rho_{\alpha\beta}^0(t) = \begin{pmatrix} 1 - \frac{\Delta^2}{E_0^2} \sin^2 E_0 t & -i \frac{\Delta}{E_0} \sin E_0 t \\ i \frac{\Delta}{E_0} \sin E_0 t & \frac{\Delta^2}{E_0^2} \sin^2 E_0 t \end{pmatrix} \quad (3.58)$$



where the eigenenergies are

$$E_{\pm} = \pm |E_0| = \pm (\Delta^2 + \xi_0^2)^{1/2} \quad (3.59)$$

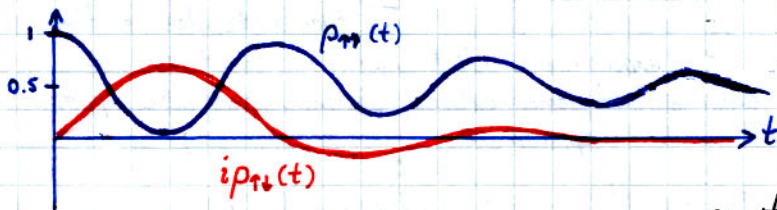
(ii) $\xi_0 \gg \Delta$



and we have assumed an initial state $|\uparrow\rangle$ for the system (and the system remains of course in a pure state thereafter). Notice that when $\xi_0 \gg \Delta$, the system is almost frozen in $|\uparrow\rangle$, even if this is the high energy state - there is no way for

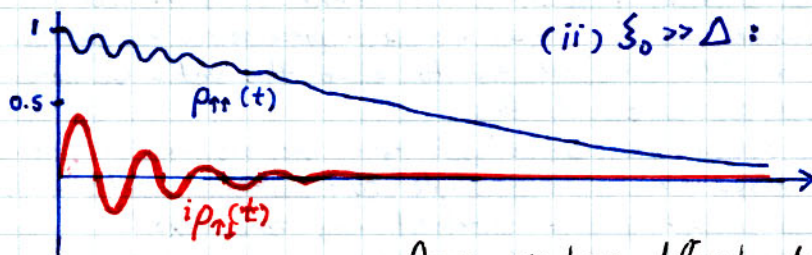
it to relax, since only an energy Δ can be provided by Δ (which is driving the transitions between $|\uparrow\rangle$ and $|\downarrow\rangle$).

Now consider what happens when we couple to an environment.



(i) $\xi_0 = 0$: In this case the diagonal matrix elements decay to values 0.5 as $t \rightarrow \infty$; this is obvious

because the 2 states are degenerate. Note there is no reason to believe that the diagonal and non-diagonal elements should damp out at the same rate! If the environment couples to \hat{c}_z , then it will preferentially damp $\rho_{12}(t)$.



(ii) $\xi_0 \gg \Delta$: In the presence of any finite bias the system will eventually relax to the lowest state (here it relaxes to $|\downarrow\rangle$).

Again, we have different characteristic times. In

fact we see there are decoherence times for the oscillations, and also there are relaxation times - here, it takes $\rho_{pp}(t)$ a long time to relax, long after all interference has disappeared.

Note that these pictures are GUESSES - you should by now be wondering how to go beyond a guess, and see what kinds of behaviour are possible.

§4. QUANTUM PHASES - INTRO

The essence of QM is in the interference between different states, and the complex nature of these states, which can be understood in terms of a phases. For a pure state these phases are real; but for a reduced density matrix we have seen they are complex, in eqn. (3.54).

If we look at eqns like (3.18), (3.19), (3.22), (3.33), or (3.36-38) for isolated systems in pure states (with a time-independent Hamiltonian - it makes no sense for an isolated system to have a time-dependent Hamiltonian) then the phase evolution in time seems rather trivial - it just evolves linearly in time, at a rate governed by energy differences. This is usually called the DYNAMIC PHASE.

However we can ask very interesting questions about phase evolution in the presence of time-dependence in the Hamiltonian. Here we just take a first look at this fascinating subject, which is of course intimately related to the subject of entanglement.

4(a) TIME-DEPENDENT HAMILTONIANS

To even write down a time-dependent Hamiltonian implies an approximation which must be considered very carefully. It implies a coupling to some external system, and the approx. is thus that we can make the replacement

$$\hat{H} = [\hat{H}_0(1) + \hat{H}_{\text{ext}}(2) + \hat{H}_{\text{int}}(1,2)] \implies \hat{H}_0(1) + \hat{V}_0(t) \quad (4.1)$$

where $\hat{H}_0(1)$ is a renormalised but t -independent Hamiltonian for system 1, and $\hat{V}_0(t)$ is a time-dependent term acting on system 1. It is an interesting and important question (to which the answer is by no means obvious) to understand when we may make such a replacement, and what are the errors involved. We shall not try to answer this yet - we need to do a lot more before we can do this.

Note that a solution to Schrodinger's eqn. when we have a time-dependent term is not easy - even a very simple term makes it rather nasty. Because of this one often attempts a treatment using time-dependent perturbation theory, which depends for its accuracy on the slowness of the

perturbation $V(t)$. Recall how this works; there are various techniques, and we look briefly at two.

(i) TIME-DEPENDENT PERTURBATION THEORY : Starting from the TDSE in the form (3.13), we

write the solution as

$$\psi(t) = \sum_n C_n(t) \psi_n(t) \quad (4.2)$$

where the $\psi_n(t)$ are the time-dependent eigenfunctions of \mathcal{H}_0 , in (3.19). The time-dependence in $C_n(t)$ comes from the $V(t)$, of which there is an interesting part (the time-dependent part) and an uninteresting part (the constant part, which in general does not commute with \mathcal{H}_0). To lowest order we find

$$\left. \begin{aligned} C_n(t) &= \hat{T}_{nm}(t) C_m(0) \\ T_{nm}(t) &= -\frac{i}{\hbar} \int dt' V_{nm}^0(t') e^{i\Omega_{nm}t'} \end{aligned} \right\} \quad (4.3)$$

where $V_{nm}^0(t) = \langle n | \hat{V}_0(t) | m \rangle$. The interesting part appears if we integrate by parts to get, for the transition matrix element:

$$T_{nm}(t) = \frac{1}{\hbar} \int dt' \frac{e^{i\Omega_{nm}t'}}{\Omega_{nm}} \frac{\partial V_{nm}^0(t')}{\partial t'} - \frac{1}{\hbar} \left[V_{nm}^0(t') \frac{e^{i\Omega_{nm}t'}}{\Omega_{nm}} \right]^t \quad (4.4)$$

where the 2nd part is just the time-dependence coming from the level shift, and is of no interest (we see that it is just the usual expression coming from time-independent perturbation theory, with energy denominator

$$\Omega_{nm} = E_n - E_m \quad (4.5)$$

Thus from (4.4) we get a transition probability, between the UNPERTURBED STATES (not counting the t -dependence) given by

$$W_{nm}(t) = |T_{nm}(t)|^2 = \frac{1}{\hbar^2} \left| \int dt' \frac{\partial V_{nm}^0(t')}{\partial t'} \frac{e^{i\Omega_{nm}t'}}{\Omega_{nm}} \right|^2 \quad (4.6)$$

From this we see that $W_{nm} \sim O(|V_{nm}^0|^2 / \Omega_{nm}^2)$, and so is small for quasi-adiabatic perturbation, provided the total change $\ll \Omega_{nm}$. However this result is a little misleading...

(ii) PERTURBATIONS IN THE ADIABATIC BASIS : The adiabatic basis of the time-dependent

Hamiltonian $\mathcal{H}(t) = \mathcal{H}_0 + V_0(t)$ is given by the solutions to the time-INDEP. eqns

$$\mathcal{H}(t=u) \chi_n^u = E_n^u \chi_n^u \quad (4.7)$$

The crucial difference now is that provided $V_0(t)$ changes slowly, there will be no transitions between the different states in (4.7), no matter how big the change that is finally accumulated in $\mathcal{H}(t)$. The basic

idea is that the states $\chi_m^u(t)$ "track" the states of the real $\mathcal{H}_0(t)$ as closely as possible.

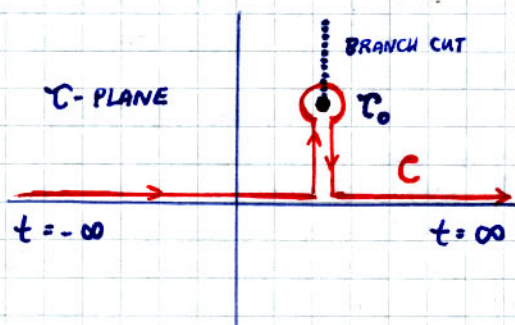
Actually, by introducing this idea we have opened the door to a quite fascinating subject - which we will only peek at here. The story goes back to the beginning at Q.M., and even before, to the subject of adiabatic changes in a Hamiltonian, and the "quasiclassical approximation".

Let's begin in 1932, with a remarkable formula derived by Landau (which for some reason is called Dykhne's formula in the recent literature). To appreciate the formula, let's consider the problem where $\mathcal{H}_0(t)$ has a 2-d Hilbert space, i.e., it is a TLS with time-dependent parameters; in general we have

$$\mathcal{H}_0(t) = \underline{y}(t) \cdot \hat{\underline{C}} \quad (4.8)$$

We assume that the adiabatic basis has t -dependent eigenvalues $E_1(t)$ and $E_2(t)$, and then ask - what is the transition probability between the 2 levels, as we vary t from $-\infty$ to ∞ ? The result found by Landau was

$$\tilde{W}_{21} \sim \exp \left\{ -2 \int_C \text{Im} \int_{\tau_0}^{\tau_0} d\tau (E_2(\tau) - E_1(\tau)) \right\} \quad (4.9)$$



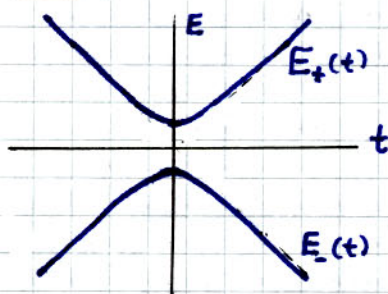
where the integration path from $-\infty < t < \infty$ is taken along the contour shown - this is because the functions $E_1(\tau)$ and $E_2(\tau)$ are expected to cross somewhere in the complex time plane, and the point τ_0 satisfies the equation

$$E_2(\tau) - E_1(\tau) \Big|_{\tau=\tau_0} = 0 \quad (4.10)$$

and in fact in a 2-level problem like this, there is typically a square-root approach of $E_2 - E_1$ towards zero as one approaches τ_0 (so that the point τ_0 is the end point of a branch cut in the complex plane). There are various ways to demonstrate this formula (and how accurate it might be), but we won't do this just yet.

It is useful to consider an example at this point - so we take a special case:

Example: Let us take the "Landau-Zener" model, in which the t -dependent Hamiltonian is



$$\mathcal{H}_0(t) = \Delta \hat{\tau}_x + vt \hat{\tau}_z \quad (4.11)$$

$$= \begin{pmatrix} vt & \Delta \\ \Delta & -vt \end{pmatrix} \quad (4.12)$$

with adiabatic levels $E_{\pm}(t)$ shown - these

are just given by

$$E_{\pm}(t) = \pm |E_0(t)| = \pm (\Delta^2 + v^2 t^2)^{1/2} \quad (4.12)$$

(cf. (3.59)). The levels cannot cross in real time, but in complex time we find

$$E_+(t) - E_-(t) \Big|_{t = i \frac{\Delta}{v}} = 0 \quad (4.13)$$

and so the integral in (4.9) becomes

$$\begin{aligned} \tilde{w}_{\pm} &\sim \exp \left\{ -\frac{1}{2} g_m \int_0^{i \Delta/v} dt (\Delta^2 + v^2 t^2)^{1/2} \right\} \\ &= e^{-\pi \Delta^2/v} \end{aligned} \quad (4.14)$$

In reality we have no particular reason to expect (4.14) to be exact, since (4.9) is an asymptotic result, correct in the limit that

$$\lambda_n \sim \dot{E}_n / \Delta E_n \ll 1 \quad (4.15)$$

where \dot{E}_n is the rate of change of E_n with t , and ΔE_n is the distance of nearest approach of the other adiabatic levels to $E_n(t)$. One then expects that

$$\tilde{w}_{21} \sim e^{-A/\lambda} \quad (4.16)$$

where $A \sim O(1)$. However in fact, for the LZ Hamiltonian (4.11), the result (4.14) is exact, no matter how fast the transition (i.e., no matter how large is v). This can be shown by solving (4.11) exactly, a formidable task first performed by Zener in 1932; one has to solve the pair of eqns

$$\left. \begin{aligned} vt \psi_{\uparrow}(t) + \Delta \psi_{\downarrow}(t) &= i \hbar \partial_t \psi_{\uparrow}(t) \\ \Delta \psi_{\uparrow}(t) - vt \psi_{\downarrow}(t) &= i \hbar \partial_t \psi_{\downarrow}(t) \end{aligned} \right\} \quad (4.17)$$

which has disgustingly complex solution in terms of parabolic cylinder functions.

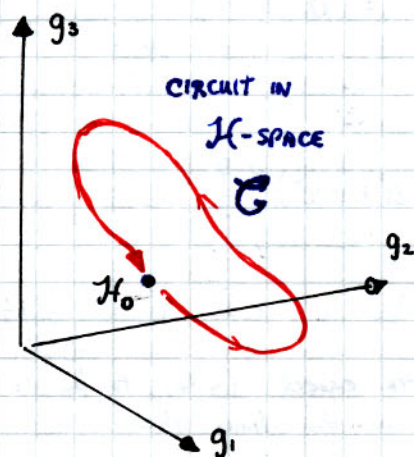
Note that in general there will be more than one crossing point, particularly if there is more than one other level - then we take the one for which τ_0 makes the closest approach to the real axis. The whole problem is then an exercise in asymptotic analysis.

Now, the crucial result in our problem appears in (4.16), that the transition probability between adiabatic levels is EXPONENTIALLY SMALL in $\partial V / \partial t$. This is much smaller than the quadratic dependence on $\partial V / \partial t$ for transitions between the unperturbed levels. As $\partial V / \partial t \rightarrow 0$, the Landau formula (4.9) [which is easily generalised to multiple levels] becomes exact.

However, this is not all that one can say about all of this

4(b) THE BERRY PHASE

From the preceding discussion you might think that, provided one accepts a formula like (4.9) (remember, we have not demonstrated this yet), then the adiabatic limit (as $\partial V/\partial t \rightarrow 0$) is really very simple. However there is a further surprise. Let's now consider a general Hamiltonian $\mathcal{H}(t)$, and cycle it around Hamiltonian space according to the following procedure:



$$\begin{aligned} \mathcal{H}(t) &= \mathcal{H}_0 + V(t) \\ &= \mathcal{H}(\underline{g}(t)) \end{aligned} \quad (4.18)$$

$$\text{with } V(t) = 0 \quad \left. \begin{array}{l} t < 0 \\ t > T. \end{array} \right\} \quad (4.19)$$

We have parametrized $\hat{V}(t)$ by a set of couplings $\underline{g}(t) = (g_1(t), g_2(t), \dots, g_N(t))$, which are shown as 3-d in the diagram. We define the adiabatic states as before:

$$\mathcal{H}(\underline{g}) |n(\underline{g})\rangle = E_n(\underline{g}) |n(\underline{g})\rangle \quad (4.20)$$

where $|n(\underline{g})\rangle = |\chi_n(\underline{g}(t))\rangle$ in the notation in (4.7).

Now in the adiabatic limit where $\dot{\underline{g}} \rightarrow 0$ we know that a system starting in one of the eigenstates $|n_0\rangle \equiv |\psi_n\rangle$ of \mathcal{H}_0 will finish in this state when $t > T$. But let's look at its t -dependence. Let us substitute the form

$$\psi(t) = |n(\underline{g}(t))\rangle e^{-i\phi_n(t)} \quad (4.21)$$

$$\text{into Schrödinger's eqn } \hat{\mathcal{H}}(t) \psi(t) = i\hbar \partial_t \psi(t) \quad (4.22)$$

$$\text{with initial condition } \psi(t=0) = \psi_n \equiv |n_0\rangle \quad (4.23)$$

We then find, following Berry, that

$$\phi_n(t) = \phi_{\text{dyn}}^n(t) + \phi_B^n(t) \quad (4.24)$$

$$\text{where } \dot{\phi}_{\text{dyn}}^n(t) = \frac{1}{\hbar} E_n(\underline{g}(t)) \quad (4.25)$$

$$\dot{\phi}_B^n(t) = i \dot{\underline{g}}(t) \cdot \langle n(\underline{g}(t)) | \partial / \partial \underline{g} n(\underline{g}(t)) \rangle \quad (4.26)$$

so that

$$\phi_{\text{dyn}}^n(t) = \frac{1}{\hbar} \int_0^t dt' E_n(\underline{g}(t')) \quad (4.27)$$

but

$$\phi_B^n(t) = i \oint_C d\underline{g} \cdot \langle n(\underline{g}) | \nabla_{\underline{g}} n(\underline{g}) \rangle \quad (4.28)$$

Now the dynamical phase we have seen before - it is just a measure of the integrated frequency oscillations around the circuit. What (4.24) tells us is that there is an extra contribution, over and above the integrated frequency oscillations. This "Berry phase" depends only on the form of the circuit \mathcal{C} in Hamiltonian space!

In this Hamiltonian space we can use a "Stokes's theorem" to rewrite ϕ_B as

$$\phi_B(\tau) \equiv \phi_B(\mathcal{C}) = - \oint_{\mathcal{C}} d\underline{S}_g \cdot \underline{b}_n(g) \quad (4.29)$$

$$\begin{aligned} \text{where} \quad \underline{b}_n(g) &= \mathcal{I}_m (\nabla_g \times \langle n(g) | \nabla_g n(g) \rangle) \\ &\equiv \mathcal{I}_m \langle \nabla_g n | \times | \nabla_g n \rangle \end{aligned} \quad (4.30)$$

which can be written in a form noted earlier in special cases by various authors working on particular problems in the form

$$\underline{b}_n(g) = \mathcal{I}_m \sum_{m \neq n} \frac{\langle n(g) | \nabla_g \hat{H}(g) | m(g) \rangle \times \langle m(g) | \nabla_g \hat{H}(g) | n(g) \rangle}{(E_n(g) - E_m(g))^2} \quad (4.31)$$

where we note that

$$\langle m(g) | \nabla_g n(g) \rangle = \frac{\langle m | \nabla_g \hat{H} | n \rangle}{E_n - E_m} \quad (4.32)$$

and insert intermediate states $|m\rangle\langle m|$ into (4.30).

This result tells us that there is a "hidden geometry" in Hamiltonian space, whose effects appear if one moves a physical system around in this space. We are beginning to see that both Hilbert space and Hamiltonian space are full of interesting underlying structure. In fact if we let $\underline{b}_n(g)$ be a "field" in \mathcal{H} -space, so that ϕ_B is a flux, and so that $\underline{b}_n(g) = \nabla_g \times \underline{\phi}_n^B$, we will not be surprised to learn that if instead of a single state $|n\rangle$ we deal with a set of degenerate states $|n_\mu\rangle$, $\mu = 1, 2, \dots, p$, then we can generalise to

$$\left. \begin{aligned} \psi(t) &= \hat{U}^{\mu\nu}(t) |n_\nu(g(t))\rangle \\ \hat{U}^{\mu\nu}(t) &= e^{-i(A_{dyn}^{\mu\nu}(t) + A_B^{\mu\nu}(t))} \end{aligned} \right\} \quad (4.33)$$

$$\left. \begin{aligned} \underline{A}_B^{\mu\nu}(g) &= i \langle n^\mu(g) | \nabla_g | n^\nu(g) \rangle \\ \underline{B}_B^{\mu\nu}(g) &= \nabla_g \times \underline{A}^{\mu\nu} - i(\underline{A} \times \underline{A})^{\mu\nu} \end{aligned} \right\} \quad (4.34)$$

ie., we deal with a non-Abelian ($SU(p)$) generalisation of the Berry

phase, with a corresponding generalisation of the underlying "field".

Actually this Hamiltonian space geometry is quite interesting, but before we start getting too abstract, let's consider some examples:

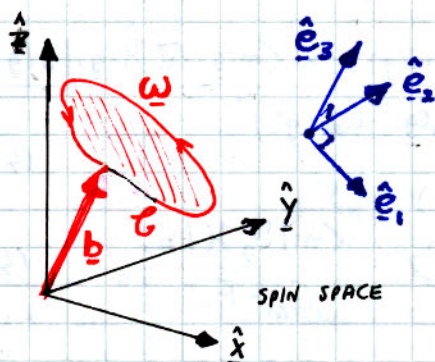
(i) BERRY PHASE FOR A TLS: We start with our favourite 2-level system, with the Hamiltonian in the form (4.8); without loss of generality we pick $\gamma = 1$ (incorporating it into the defⁿ of \underline{b}), so that

$$\hat{H}_0 = \underline{b}(t) \cdot \hat{\tau} \quad (4.35)$$

and choose our 2 adiabatic states as those quantized along the instantaneous \underline{b} axis:

$$\{ |n(\underline{b}(t))\rangle \} \rightarrow \begin{array}{ll} |+\rangle & \hat{H}|+\rangle = |\underline{b}| |+\rangle \\ |-\rangle & \hat{H}|-\rangle = -|\underline{b}| |-\rangle. \end{array}$$

(cf. (4.11), which is a special case of this in which $b_y = 0$ always).



We assume τ both for our coupling vector \underline{b} ($\equiv \underline{g}$); in fact \underline{b} is a vector in spin space, not real space. We can define instantaneous axes ($\hat{e}_1, \hat{e}_2, \hat{e}_3$), and in this frame we have $|\underline{b}| = b_3$, since \hat{e}_3 is the instantaneous axis of quantization.

Let us now calculate the Berry phase for a system which at $t=0$ is in the state $|+\rangle$ along some reference axis. We wish to find the

phase ϕ_B^+ , accumulated after a circuit \mathcal{C} in \underline{b} -space. From (4.29) and (4.34) this is given by

$$\phi_B^+(\mathcal{C}) = -\oint_{\mathcal{C}} d\underline{S}_b \cdot \underline{b}_+(\underline{b}(t)) \quad (4.36)$$

with

$$\underline{b}_+(\underline{b}) = g_m \left\{ \frac{\langle +(\underline{b}) | \nabla_{\underline{b}} \mathcal{H}_0(\underline{b}) | -(\underline{b}) \rangle \times \langle -(\underline{b}) | \nabla_{\underline{b}} \mathcal{H}_0(\underline{b}) | +(\underline{b}) \rangle}{(E_+(\underline{b}) - E_-(\underline{b}))^2} \right\} \\ \rightarrow g_m \left\{ \frac{\langle + | \hat{\tau} | - \rangle \times \langle - | \hat{\tau} | + \rangle}{4b^2} \right\} \quad (4.37)$$

where we simply use $\nabla_{\underline{b}} (\underline{b} \cdot \hat{\tau}) = \hat{\tau}$. Now we see why the cross product is important, because $\hat{\tau}_1 \times \hat{\tau}_2$ is not zero. Using $\hat{\tau}_{\pm} = \frac{1}{2}(\hat{\tau}_1 \pm i\hat{\tau}_2)$, we then get

$$\underline{b}_+(\underline{b}) = g_m \left\{ \frac{4i\hat{e}_3}{4b^2} \right\} = \frac{b}{b^3} \hat{e}_3 = \frac{1}{b^2} \hat{b} \quad (4.38)$$

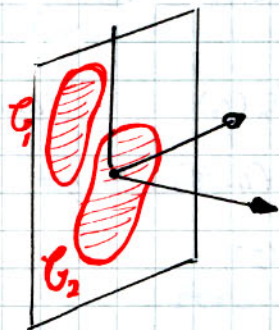
From this result we immediately see that $\vec{L}_\pm(\underline{b})$ is nothing but the field from a "monopole" in \underline{b} -space, with unit strength. If we then do the integration in (4.36), we find

$$\phi_B^+(\mathcal{C}) = -\omega \quad (4.39)$$

where $\omega = |\omega|$ is the area of the circuit (the SOLID ANGLE) seen from the origin (in \underline{b} -space). Likewise one finds

$$\phi_B^-(\mathcal{C}) = +\omega. \quad (4.40)$$

It is actually interesting to now go to the special case where the circuit is only in a plane which cuts the origin. How do we then decide what is the solid angle? If the circuit encircles the origin it is not at all obvious what is the answer to this - we can easily argue that half of the unit sphere is being covered. This is correct, and so one finds that



$$\left. \begin{aligned} \phi_B(\mathcal{C}_2) &= \pm 2\pi && \text{(ORIGIN ENCLOSED)} \\ \phi_B(\mathcal{C}_1) &= 0 && \text{(ORIGIN NOT ENCLOSED)} \end{aligned} \right\} (4.41)$$

Notice that the sign ambiguity in (4.41) for $\phi_B(\mathcal{C}_2)$ is not important, because one still has

$$e^{i\phi_B(\mathcal{C}_2)} = -1 \quad (4.42)$$

no matter which choice we make. Notice that this special case corresponds to the THS Hamiltonian we have been discussing extensively up until now (cf. (3.57), for example, or (4.11)).

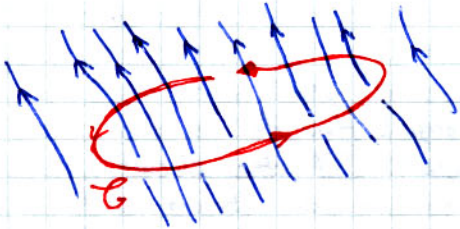
Now let us stand back and recall that (4.35) doesn't necessarily describe a spin in a field. It describes ANY quantum system near a point of ACCIDENTAL DEGENERACY (i.e., one not forced by symmetry). That we need to have 3 parameters (b_x, b_y, b_z) to find this point is a corollary of an interesting result for Hermitian matrices due to von Neumann & Wigner, at the very beginning of QM, viz., that "degeneracies (accidental) have co-dimension 3" for Hermitian matrices. If we can only vary 2 parameters (as for the Hamiltonian in (3.57) or (4.11)) then we can't find this degeneracy.

In the case where there is already degeneracy forced on the levels by symmetry, we go to the case of the non-Abelian Berry phase (cf. (4.33), (4.34)). This generalization for a "spin" already leads us to the idea of a non-Abelian monopole - it is very useful in molecular physics as well as high-energy physics.

(ii) THE AHARONOV-BOHM EFFECT : Let's now consider a particle with "CHARGE" q , coupled to a vector gauge field $A(r)$. The charge is, by defⁿ, simply the strength of this coupling, and the relevant coupling is obtained by the "minimal substitution"

$$\underline{p} \rightarrow \underline{p} + qA(r) \quad (4.43)$$

in whatever is the Hamiltonian in the absence of this coupling. Consider now the situation shown in the figure where C is a circuit in real space, in a region where flux may or may not exist



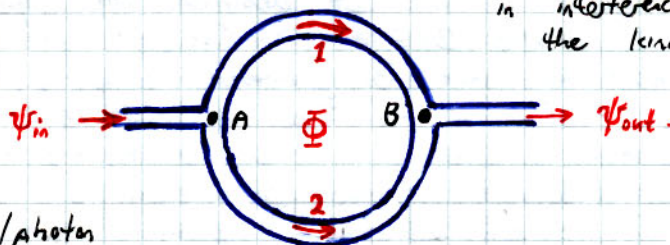
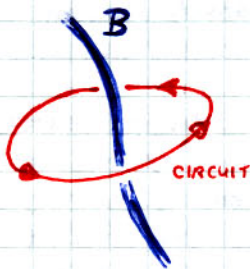
The problem is conveniently treated by taking the coupling to be the position itself - or rather, the variable parameter involved in the coupling. The coupling (4.43) immediately gives adiabatic states

$$\langle r_0 | \pi(r) \rangle = e^{-i \frac{q}{\hbar} \int_{r_0}^r A(r') \cdot dr'} \psi_n(r_0) \quad (4.44)$$

and then we can compute $\phi_B(C)$ directly from (4.28), to get

$$\begin{aligned} \phi_B &= \oint_C \langle \pi(r) | \nabla_r | \pi(r) \rangle = \frac{q}{\hbar} \oint_C dr \cdot A(r) \\ &= \frac{q}{\hbar} \Phi \end{aligned} \quad (4.45)$$

where Φ is the flux enclosed by C . The crucial point made by Aharonov & Bohm (see also Ehrenberg & Sidisy) is that there is no need for the particle to ever pass through a region where field is finite. Thus the situation shown at left, with field confined to a tube, also gives a finite accumulated phase. The physical effect of this phase can be seen in interference expts of the kind shown



We send a particle / photon in, and divide its path, so that the outgoing wave-function becomes

$$\psi_{out}(\Phi) = \left[\psi_1 e^{-i \frac{q}{\hbar} \int_0^L A(r_1) \cdot dr_1} + \psi_2 e^{-i \frac{q}{\hbar} \int_0^L A(r_2) \cdot dr_2} \right] \quad (4.46)$$

where the integrals are taken along paths 1 and 2 in the diagram, up to point B at distance L from A. Then we immediately find that

$$\begin{aligned}
 |\psi_{\text{out}}|^2 &= |\psi_1|^2 + |\psi_2|^2 + 2 \operatorname{Re}(\psi_1^* \psi_2 e^{i \frac{q}{\hbar} \oint_C A(\mathbf{r}) \cdot d\mathbf{r}}) \\
 &= |\psi_1|^2 + |\psi_2|^2 + 2 |\psi_1| |\psi_2| \cos \frac{q}{\hbar} \Phi \quad (4.47)
 \end{aligned}$$

where \mathcal{C} is the entire circuit around the ring. This effect was initially received with incredulity, but is now basic to mesoscopic and macroscopic quantum phenomena.

Again, one generalise these considerations to non-Abelian gauge fields, in the same way as discussed before.

REFERENCES for LECTURE 2

** For the relevant classical mechanics, see **LL1**, particularly sections §2, 43, and 51; and various articles in **Wile**.

** For the relevant Q.M., see **Sch**, **Fey3**, and **Fey1**. The book by Schiff is also useful. For path integrals see the same books.

** For the treatment of the density matrix using the influence functional, see **Fey1**, last chapter, as well as the following articles:
 R.P. Feynman, F.L. Vernon, *Ann. Phys.* 24, 118 (1963)
 A.J. Leggett et al., *Rev. Mod. Phys.* 59, 1 (1987)
 N.V. Prokof'ev, PCE Stamp, *Rep. Prog. Phys.* 63, 669 (2000)
 A lot more detail is also in **Weiss** and **Toms**.

** For the discussion of the Berry phase, the original paper is essential reading:

M.V. Berry, *Proc. Roy. Soc.* A392, 45 (1984)

This and other important papers (including anticipations of the Berry phase) are reprinted in **Wile**. The classic flux phase was discovered in

Y. Aharonov, D. Bohm, *Phys. Rev.* 115, 485 (1959)

which is also essential reading.

** The problem of quasi-adiabatic levels, and transitions between them, was first addressed by Landau in 1932, in
 L.D. Landau *Phys. Z. Sowjet.* 1, 89 (1932)
 and is discussed in **LL3**, section §52, 53 (see also **LL1**, §51); the application to the Landau-Zener problem appears here. This problem was also solved by

C. Zener, *Proc. Roy. Soc.* A137, 696 (1932)

E.G.C. Stückelberg, *Helv. Phys. Acta* 5, 369 (1932)

and is also discussed by various writers in **Wile**. The Wigner-von Neumann theorem is in

J. von Neumann, *EP Wigner* *Z.f. Physik* 30, 467 (1929)