A.3. INTRO TO PATH INTEGRALS

In the relatively few texts that do present the path integral formulation of quantum mechanics, it is somewhat divorced from the more traditional presentations. This is a pity, since the complex of relationships between the traditional point of view, the path integral formulation, and related semiclassical techniques is very fruitful. In what follows we will make some of these links. We will begin by giving the basic formulation, and relating it back to Schrödinger's eqtn. We then look briefly at some elementary results derived using path integral theory. Finally, we show how one also formulates the dynamics of density matrices in this language.

A.3.1. BASIC FORMULATION

There are several ways to formulate path integral theory. One is to derive it, in a fairly unwieldy way, from the conventional formulation of Q.M. This is tedious & also somewhat artificial. The second is to simply postulate it, and then show that one recovers the traditional formulation for simple systems. This has the advantage that one can extend this postulate to systems for which the traditional formulation is hard to implement (eg., in quantum field theory). We will look at these two formulations, and ignore any others.

A.3.1.(a) THE IDEA OF A PROPAGATOR

: In Q.M. we often have to deal with the problem of finding the "transition amplitude" for a system to go from state $|\psi_\alpha(t_1)\rangle$, at time t_1, to state $|\psi_\beta(t_2)\rangle$ at some other time t_2 (which will assume to be later for convenience. Now from (109) we can clearly write

$$|\psi(t_2)\rangle = e^{-i/\hbar \hat{H}(t_2-t_1)}|\psi(t_1)\rangle \qquad (213)$$

and if we project onto the eigenstates of $\hat{H}$, writing

$$\hat{H}|n\rangle = \epsilon_n|n\rangle \qquad (214)$$

we have

$$|\psi_n(t_2)\rangle \equiv |n(t_2)\rangle = e^{-i/\hbar \epsilon_n(t_2-t_1)}|n(t_1)\rangle \qquad (215)$$

Now define the operator

$$\left.\boxed{\begin{aligned}\hat{G}(t_2-t_1) &= e^{-i/\hbar\hat{H}(t_2-t_1)} \\ &= \sum_n |n\rangle e^{-i/\hbar\epsilon_n(t_2-t_1)}\langle n|\end{aligned}}\right\} \qquad (216)$$

which is diagonal in the energy eigenstate representation, ie.

$$\left.\begin{aligned}\langle n|\hat{G}(t_2-t_1)|n\rangle &= G_{nn}(t_2-t_1) \\ &= e^{-i/\hbar\epsilon_n(t_2-t_1)}\end{aligned}\right\} \qquad (217)$$

but not in the position representation:

$$G(r_2,r_1;t_2-t_1) = \langle r_2|\hat{G}(t_2-t_1)|r_1\rangle = \sum_n \langle r_2|n\rangle e^{-i/\hbar\epsilon_n(t_2-t_1)}\langle n|r_1\rangle \qquad (218)$$

The operator $\hat{G}$ is of course just the time evolution, but it is often called the "propagator" operator; and the function $G_{\beta\alpha}(t_2-t_1)$, given by

$$G_{\beta\alpha}(t_2-t_1) = \langle\beta|\hat{G}(t_2-t_1)|\alpha\rangle \qquad (219)$$

is called the "propagator", or "transition amplitude", or "1-particle Green function" for the system, from state $|\alpha\rangle$ to state $|\beta\rangle$. The function $G(\underline{r}_2,\underline{r}_1;t_2-t_1)$ is then the propagator, or 1-particle Green function, from a "position" $(\underline{r}_1,t_1)$ to position $(\underline{r}_2,t_2)$, in spacetime; transition amplitude is also often just called the "amplitude".

By taking the Hilbert space product of $|\psi\rangle$ in (213) with $\langle\underline{r}|$, we can write

$$\begin{aligned}\langle r|\psi(t_2)\rangle &= \langle\underline{r}|\hat{G}(t_2-t_1)|\psi(t_1)\rangle \\ &= \langle r|\hat{G}(t_2-t_1)|\underline{r}'\rangle\langle\underline{r}'|\psi(t_1)\rangle\end{aligned} \qquad (210)$$

ie., that

$$\boxed{\psi(r,t_2) = \int d^3r'\; G(\underline{r},\underline{r}';t_2-t_1)\;\psi(\underline{r}',t_1)} \qquad (211)$$

where

$$\left.\begin{aligned}G(\underline{r},\underline{r}';t_2-t_1) &= \langle\underline{r}|\hat{G}(t_2-t_1)|r'\rangle \\ &\equiv \langle\underline{r}|n\rangle\langle n|\hat{G}(t_2-t_1)|n\rangle\langle n|\underline{r}'\rangle\end{aligned}\right\} \qquad (212)$$

which we write out explicitly as

$$\boxed{G(r,r';t_2-t_1) = \sum_n \psi_n(r)\psi_n^*(r')\, e^{-i/\hbar\,\epsilon_n(t_2-t_1)}} \qquad (213)$$

Recalling that we get (213) from the Schrodinger eqtn purely by integrating it up, we notice that we can also rewrite the definition of $\hat{G}$ in differential form, ~~as~~ either the operator form or in a specific representation:

$$\boxed{(\hat{\mathcal{H}} - i\hbar\,\partial_t)\,\hat{G}(t,t') = -i\hbar\,\hat{\mathbf{1}}\,\delta(t-t')} \qquad (214)$$

or, in the position representation:

$$\left.\begin{aligned}(\mathcal{H} - i\hbar\partial_t)\langle\underline{r}|\hat{G}(t,t')|\underline{r}'\rangle &= -i\hbar\langle\underline{r}|\hat{\mathbf{1}}|\underline{r}'\rangle\,\delta(t-t') \\ &\equiv -i\hbar\,\delta(\underline{r}-\underline{r}')\,\delta(t-t')\end{aligned}\right\} \qquad (215)$$

These results are a straightforward application the theory of ordinary differential equations - the definition of a Green function for the differential operator $\hat{L} = \mathcal{H}_0 - i\hbar\partial_t$ in the form (214) is standard, and immediately implies the integral relation (211). Note that time is treated as a parameter in (214), quite differently from space - it is not legitimate in ordinary QM to imagine sandwiching the unit operator $\hat{\mathbf{1}}$ between "time eigenstates" to produce the $\delta(t-t')$ term.

It is useful to Fourier transform these relations from time to frequency space. We write

$$\left.\begin{aligned}\hat{G}(\omega) &= \int dt\, e^{i\omega t}\,\hat{G}(t) \\ &= \int dt\, e^{i(\omega - \hat{\mathcal{H}}/\hbar)t}\end{aligned}\right\} \qquad (216)$$

which gives

$$\boxed{\hat{G}(\omega) = \frac{i}{\omega - \hat{\mathcal{H}}/\hbar}} \qquad (217)$$

with matrix elements

$$\langle\beta|\hat{G}(\omega)|\alpha\rangle = \sum_m \langle\beta|m\rangle\frac{1}{\omega - \epsilon_m/\hbar}\langle m|\alpha\rangle \qquad (218)$$

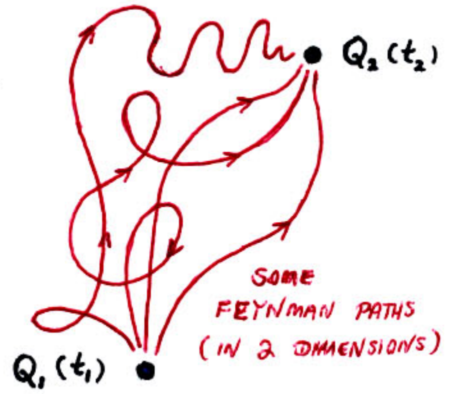
so that in particular

$$\langle\underline{r}|\hat{G}(\omega)|\underline{r}'\rangle = G(r,r';\omega) = \sum_m \frac{\psi_m^*(r)\,\psi_m(r)}{\omega - \epsilon_m/\hbar} \qquad (219)$$

These forms are general - later, in the discussion of scattering theory, and other problems involving interactions, we will see how useful it is to make ω a complex variable.

A.3.1.(b) PATH INTEGRAL FORM for $\hat{G}_{\beta\alpha}$:

Now let us introduce the remarkable Feynman form for the propagator. This is inspired very much by the idea of paths in configuration space which is at the core of the classical least action principle.



Let us consider the amplitude for a system to go from a state $|Q_1(t_1)\rangle$ to $|Q_2(t_2)\rangle$; we revert here to the notation Q, Q', etc., because we are going to be dealing in general with systems of many particles - so $Q = (\underline{r}_1, \underline{r}_2, \dots \underline{r}_N)$.

The basic formula of path integral theory states that

$$\boxed{G(Q_2, Q_1; t_2, t_1) = \int_{q(t_1)=Q_1}^{q(t_2)=Q_2} \mathcal{D}q(\tau)\, e^{i/\hbar\, S[q,\dot{q}]}} \qquad (220)$$

where, as usual
$$S[q,\dot{q}] = \int_{t_1}^{t_2} dt\, L(q\dot{q};t) \qquad (221)$$

The meaning of this formula is defined by the path integration: $\int \mathcal{D}q(\tau)$, with its associated measure, which we discuss in more detail below. The basic idea is that we sum over all possible paths between $Q_1(t_1)$ and $Q_2(t_2)$, as shown in the figure. Each path in the sum is weighted by a factor

$$W_\mu = e^{i\varphi_\mu} = \exp\left\{ \frac{i}{\hbar} \int_{t_1}^{t_2} d\tau\, L(q_\mu(\tau), \dot{q}_\mu(\tau), \tau) \right\} \qquad (222)$$

for the "μ-th path" $q_\mu(\tau)$; and then we sum over all these paths. That some such formula might exist might have been guessed even by 19th-century physicists interested in optics, if they had investigated seriously the extraordinarily complex interference fringes one finds near caustics in light diffraction. In a certain sense (220) is a generalisation of the remarkable picture published by Huyghens in 1690, to describe wave propagation (the "Huyghens construction").

Now let us consider what is really meant by the path integration measure $\mathcal{D}q(\tau)$. A simple construction for the propagation of a single particle is to construct the paths from infinitesimal straight line segments (see diagram on next page). While this is crude, it is nothing but the usual Riemann measure for integration. Each infinitesimal segment must be integrated over the entire space the system moves in, ie., we allow arbitrarily large excursions for each infinitesimal segment (NB: this is clearly impossible in a relativistic theory). In this way one finds a priori that the set of all possible paths will be completely dominated by extremely irregular paths, fluctuating wildly over the entire space. How reasonable this is we discuss immediately below.

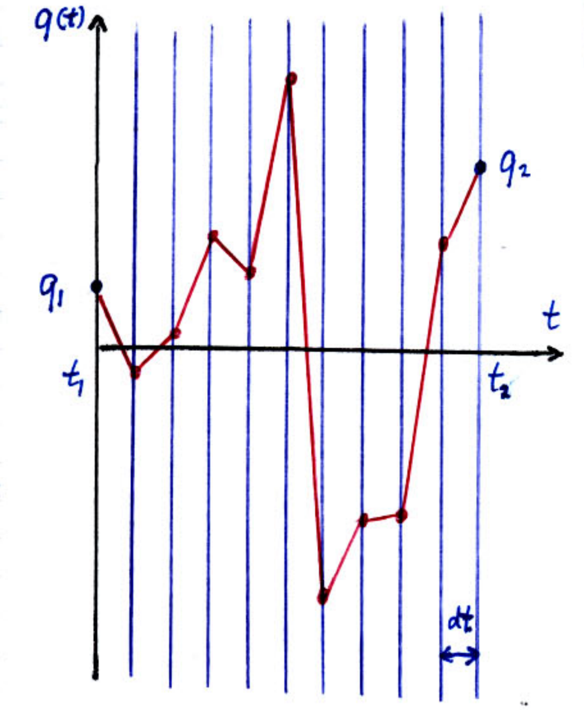
We can, using this construction of straight line segments, give a meaning to (220) ; it now becomes, using the following definitions:

and in 1 dimension:
$$dt = \frac{t_2 - t_1}{N} \qquad dx_j = x_{j+1} - x_j \qquad (223)$$

$$G(x_2 x_1; t_2, t_1) = \lim_{\substack{N \to \infty \\ dt \to 0}} \prod_{j=1}^{N-1} \int dx_j\, A_N \exp\left\{ \frac{i}{\hbar} dt \sum_{j=1}^{N-1} \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{dt} \right)^2 - V(x_j) \right] \right\} \qquad (224)$$

where the normalisation factor A_N, as we will see, is
$$A_N = \left(\frac{m}{2\pi i \hbar\, dt} \right)^{N/2} \qquad (225)$$

where we have written $Q_2 \to x_2$, $Q_1 \to x_1$ for this 1-d problem. Eqtn (224) is an obvious infinitesimal version of (220), except for the measure A_N. The restriction on the initial & final positions for the paths is not written explicitly in this formula, but is implied.



A TYPICAL PATH, MADE FROM STRAIGHT LINES

Now let us consider how to derive these formulae. The easiest way is to start from the basic expression (216) for $\hat{G}(t_2,t_1)$, and take the position matrix element & chop it into infinitesimals:

$$\left.\begin{aligned} G(r_2 r_1; t_2, t_1) &= \langle r_2 | e^{-\frac{i}{\hbar}\hat{\mathcal{H}} t} | r_1 \rangle \\ &= \langle r_2 | \left(e^{-\frac{i t}{\hbar N}\hat{\mathcal{H}}}\right)^N | r_1 \rangle \end{aligned}\right\} \quad (226)$$

and then, using (223) as before, we write this in a "Trotter product" form

$$\left.\begin{aligned} G(r_2 r_1; t_2 t_1) &= \langle r_2 | \left(e^{-\frac{i}{\hbar}\hat{T}dt} e^{-\frac{i}{\hbar}\hat{V}dt}\right)^N | r_1 \rangle \\ &= \lim_{\substack{dt\to 0\\ N\to\infty}} \prod_{j=1}^{N-1} \int dx_j \langle x_{j+1} | e^{-\frac{i}{\hbar}\hat{T}dt} e^{-\frac{i}{\hbar}\hat{V}dt} | x_j \rangle \end{aligned}\right\} \quad (227)$$

where we have sandwiched states $|x_j\rangle\langle x_j|$ between each of the N terms in the product, assumed a form $\hat{\mathcal{H}} = \hat{T} + \hat{V}$ for the Hamiltonian, and also used the Baker-Hausdorf formula

$$e^{\hat{A}+\hat{B}} = (e^{\hat{A}} e^{\hat{B}}) \times (e^{1/2[\hat{A},\hat{B}]}) \quad (228)$$

applied to the operators $\hat{A} = -\frac{i}{\hbar}\hat{T}dt$ and $\hat{B} = -\frac{i}{\hbar}\hat{V}dt$ (so that the commutator is $\sim O(dt^2)$ and can be dropped).

Now the matrix elements in (227) are easily found; we have

$$\left.\begin{aligned} \langle x_{j+1} | e^{-\frac{i}{\hbar}\hat{V}dt} | x_j \rangle &= \langle x_{j+1} | x_j \rangle e^{-\frac{i}{\hbar}V(x_j)dt} \\ &\xrightarrow[dt\to 0]{} e^{-\frac{i}{\hbar}V(x_j)dt} \end{aligned}\right\} \quad (229)$$

and

$$\left.\begin{aligned} \langle x_{j+1} | e^{-\frac{i}{\hbar}\hat{T}dt} | x_j \rangle &= \langle x_{j+1} | p \rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}dt} \langle p | x_j \rangle \\ &= \frac{1}{2\pi\hbar}\int dp\, e^{\frac{i}{\hbar}p(x_{j+1}-x_j)} e^{-\frac{i}{\hbar}\frac{p^2}{2m}dt} \\ &\longrightarrow \left(\frac{m}{2\pi i\hbar\, dt}\right)^{1/2} \exp\left\{-\frac{m}{2i\hbar dt}(x_{j+1}-x_j)^2\right\} \end{aligned}\right\} \quad (230)$$

using the standard result for a Gaussian integral, viz., $\int_{-\infty}^{\infty} dx\, e^{-Ax^2+Bx} = \left(\frac{\pi}{A}\right)^{1/2} e^{B^2/4A}$ (231)

Thus we prove (225) and (225), and hence the basic result in (220) and (222). Notice how we start with $\mathcal{H} = T+V$ and end up with $L = T-V$, simply because of the factor $(1/idt)^2$ that is produced in the kinetic term by integration of the kinetic term.

Notice that it is also a simple matter to start from (224) and derive the Schrödinger eqtn. as well. The simplest way is of course work backward from (224) to (226), and then note that (226) is just the integral form of the Schrodinger eqtn. Another way is to start from (224), and write that (cf. (211))

$$\psi(r, t+\delta t) \equiv \psi(r,t) + dt\,\frac{\partial \psi}{\partial t}$$
$$= \int dr' \left(\frac{m}{2\pi\hbar\, dt}\right) \exp\left\{\frac{i}{\hbar} dt \left[\frac{m}{2}\left(\frac{r'-r}{dt}\right)^2 - V\left(\frac{r'+r}{2}\right)\right]\right\} \psi(r', t) \qquad (232)$$

and then note that only those parts of the integrand for which $|\underline{r}'-\underline{r}| \sim dx$ are infinitesimal will contribute to the integral - expanding to 1st order in dt and 2nd order in dx, one gets the Schrödinger eqtn as a difference eqtn.

Note also that we can write the path integral in phase space; using the same notation as in (220), we have

$$G(Q_2, Q_1; t_2, t_1) = \int_{q(t_1)=Q_1}^{q(t_2)=Q_2} \mathcal{D}q(\tau)\,\mathcal{D}p(\tau)\, e^{i/\hbar\, S[q,p]} \qquad (233)$$

with the Hamiltonian form of the action, ie $S[q,p] = \int_{t_1}^{t_2} d\tau\,[P\dot{Q} - \mathcal{H}\, dt]$ (234)

We will not use this form so much as (220).

Note that if we write out the path integral (233) explicitly, it becomes, in 1 dimension:

$$G(x_2, x_1; t_2, t_1) = \lim_{\substack{N\to\infty \\ dt\to 0}} \prod_{j=1}^{N-1} \int dx_j \int dp_j \left(\frac{1}{2\pi\hbar}\right)^N \exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N}\left[P_j(x_{j+1}-x_j) - \left(\frac{P_j^2}{2m} + V(x_j)\right)dt\right]\right\} \qquad (235)$$

and in fact we can recover the usual form in (224) just by doing the integral $\int dp_j$.

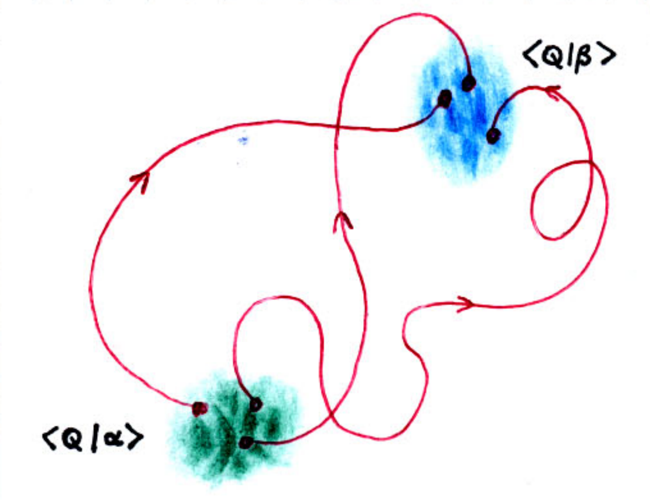
A really important point that you should take away with you is the way in which the path integral formalism has removed all reference to non-commuting variables, etc, and allows us to talk entirely in terms of classical paths for ordinary classical Hamiltonians. This turns out to be extraordinarily useful for visualising quantum processes.

There is however a catch - we need to know what is the classical Lagrangian or action if we are to do this. Feynman himself was then completely foxed by an apparently simple problem, viz.; how do we write a path integral for spin, where there is no classical Hamiltonian (spin disappears as $\hbar \to 0$)? We will see the remarkable & beautiful answer to this later in the course.

We can now summarize the path integral result for the propagation of a quantum system by asking what is the transition amplitude from a state $|\alpha(t_1)\rangle \equiv |\psi_\alpha(t_1)\rangle$ to a state $|\beta(t_2)\rangle$ at a later time t_2. This is just

$$\boxed{\langle\beta(t_2)|\alpha(t_1)\rangle = G_{\beta\alpha}(t_2 - t_1) = \int dQ_2 \int dQ_1 \langle\beta|Q_2\rangle\langle Q_1|\alpha\rangle \int_{q(t_1)=Q_1}^{q(t_2)=Q_2} \mathcal{D}q(\tau)\, e^{i/\hbar\, S[q]}} \qquad (236)$$

where we integrate over the initial and final coordinates of the path integral. This result is easily visualised (see picture on next page) as the propagation of the system from any point in one "patch" of space, represented by the amplitude $\langle Q_1|\alpha\rangle$, to another patch represented by the amplitude $\langle Q_2|\beta\rangle$; the system is allowed to propagate from any point in the first of these to any point in the second.



SOME OF THE PATHS CONTRIBUTING TO THE TRANSITION AMPLITUDE $G_{\beta\alpha}(t_2-t_1)$

So far so good. Now, what about the expectation value of operators? This is fairly easy to work out. Suppose we have some operator $\hat{A}(t)$ which for convenience we will assume to be diagonal in real space, ie.,

$$\langle Q|\hat{A}(t)|Q'\rangle = A(t)\,\delta(Q-Q'). \qquad (237)$$

Then we can simply compute the expectation value of $\hat{A}$. Let's in fact calculate something a little more general, viz., the expectation value of $A(t)$, taken at time t, under the assumption that we know that at time $t_1<t$, the system was in state $|\alpha(t_1)\rangle$; and that a later time $t_2>t$, the system is in state $|\beta(t_2)\rangle$. What then is $\langle A(t)\rangle$. The answer is

$$\left.\begin{aligned}\langle\beta(t_2)|\hat{A}(t)|\alpha(t_1)\rangle &= \int dx_2\int dx_1\,\langle\beta|x_2\rangle\langle x_2|A(t)|x_1\rangle\langle x_1|\alpha\rangle\\ &= \int dx_1\int dx_2\,\langle\beta|x_2\rangle\langle x_2|e^{-\frac{i}{\hbar}H(t_2-t)}\,\hat{A}\,e^{-\frac{i}{\hbar}H(t-t_1)}|x_1\rangle\langle x_1|\alpha\rangle\end{aligned}\right\}(238)$$

which in path integral language is just

$$\langle\beta(t_2)|\hat{A}(t)|\alpha(t_1)\rangle = \int dx_1\int dx_2\int dx\int dx'\,\langle\beta|x_2\rangle\int_{q(t)=x'}^{q(t_2)=x_2}\mathcal{D}q(\tau)\,e^{\frac{i}{\hbar}S}\,\langle x'|\hat{A}|x''\rangle\int_{q(t_1)=x_1}^{q(t)=x''}\mathcal{D}q(\tau)\,e^{\frac{i}{\hbar}S}\,\langle x_1|\alpha\rangle \qquad (239)$$

which if we assume $A(t)$ is diagonal in real space (cf. (237)) just gives

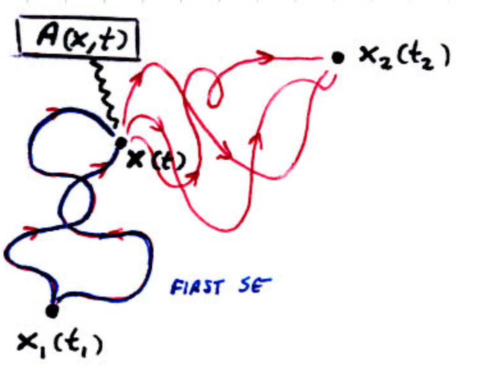
$$\langle\beta(t_2)|A(t)|\alpha(t_1)\rangle = \int dx_1\int dx_2\,\langle\beta|x_2\rangle\,G(x_2x_1;t_2t_1|A(t))\,\langle x_1|\alpha\rangle \qquad (240)$$

where we define the new Green function weighted over $A(t)$ as

$$G(x_2t_2,x_1t_1|A(t)) = \int dx\int_{q(t)=x}^{q(t_2)=x_2}\mathcal{D}q(\tau)\,e^{\frac{i}{\hbar}S[x_2,x]}\,A(x,t)\int_{q(t_1)=x_1}^{q(t)=x}\mathcal{D}q(\tau)\,e^{\frac{i}{\hbar}S[x,x_1]} \qquad (241)$$

which we write in shorthand form as

$$\boxed{G(2,1|A(t)) = \frac{\int_1^2\mathcal{D}q(\tau)\,A(t,[q])\,e^{\frac{i}{\hbar}S[q]}}{\int_1^2\mathcal{D}q(\tau)\,e^{\frac{i}{\hbar}S[q]}}} \qquad (242)$$



in which we put an integral over $e^{\frac{i}{\hbar}S}$ in the denominator to make sure the whole thing is properly normalised (so that, eg., the expectation value of the unit operator comes out to be unity).

The interpretation of (241) and (242) is shown at left – we imagine the operator $\hat{A}$ intervening at a position x at time t, and all paths must go to this intermediate spacetime point; but the space coordinate $x(t)$ is then integrated over, to produce all possible paths.

One can generalise a formula like (242) to deal with a whole string of operators if we wish. Thus the "n-point correlation function" given by

$$\langle A(t_n) B(t_{n-1}) \cdots \hat{O}(t_1) \rangle_{\beta\alpha} = \langle \beta(t) | A(t_n) B(t_{n-1}) \cdots \hat{O}(t_1) | \alpha(t') \rangle \qquad (243)$$

assuming an initial state $|\alpha(t')\rangle$ and a final state $|\beta(t)\rangle$, is given by $\langle \beta | \hat{G}_n(\hat{A}, \hat{B}, .. \hat{O}) | \alpha \rangle$ where

$$\langle \beta | \hat{G}_n(\hat{A}, .. \hat{O}) | \alpha \rangle = \frac{\int_{t'}^{t} \mathcal{D}q(\tau) \left[A(t_n) B(t_{n-1}) \ldots O(t_1) \right] e^{i/\hbar S[q]}}{\int_{t'}^{t} \mathcal{D}q(\tau) e^{i/\hbar S[q]}} \qquad (244)$$

These expressions may look a little forbidding, but the key is to realise that all we are doing is adding an extra weighting factor to the path integral - instead of the simple weighting factor W_μ for a path μ given in (222), we now have, in the expression (242) for $\langle A \rangle$, a weighting factor $A W_\mu$ for the path μ.

Finally, a brief remark on the nature of the paths one is integrating over. Even the crude straight line construction we used before tells us that we can have very wildly fluctuating paths, which are continuous but nowhere differentiable. In this case one might expect that a rigorous definition of the mathematical measure involved is rather delicate, and in fact mathematicians have had severe difficulties with these.

However there is a good reason why physicists ignore these most of the time. A path in which the direction changes suddenly is one in which an infinite force has acted (and likewise, one in which a sudden change in position occurs involves infinite velocity). Neither of these is physically meaningful, even in a non-relativistic theory. The reason is that both involve infinite energies, and thus fail to recognize that all Lagrangians and Hamiltonians used by physicists are actually "effective" ones, in which some coarse-graining in real space and (by the uncertainty principle) an upper energy cut-off is implied. Thus, it makes no sense to discuss the application of the simple Coulomb interaction Hamiltonian to a set of electrons and protons at energies of GeV, when we know that excitations quite outside the purview of this Hamiltonian dominate the physics - the Coulomb Hamiltonian is only meaningful at energies $\ll$ 1 MeV.

The key point is thus that the Hilbert space of our theory always has restrictions imposed on it, and it makes no sense to then include paths in the path integral that would involve the system passing through states outside this Hilbert space. Without going into details, we see that this means that the paths need to be smooth, with the degree of smoothness depending on the upper energy cut-off in the effective Hamiltonian. We will return to this point again, later in the course.

A.3.2. EVALUATION OF PATH INTEGRALS

Obviously path integral theory is only a curiosity unless there are easily usable methods for finding the propagators for real systems, ie., for evaluating these.

There are in fact systematic ways of doing this evaluation - the 2 main methods are

(i) An expansion about the classical path(s) [expansion in powers of $\hbar$]

(ii) Expansion in powers of a small parameter [perturbation expansion].

We will study neither of these in any detail here - the $\hbar$-expansion (also called the "semiclassical expansion") will be studied in section 4, and perturbation expansions will be studied in section 3.

What we will do here is evaluate a few simple path integrals that only require the most basic methods. This means evaluating the classical action (ie., the action along the classical path) and then looking at the effect of small fluctuations around it.

A.3.2.(a) EXPANSION ABOUT CLASSICAL PATH

: It is fairly obvious that paths near the classical path will make a very important contribution to the total propagator - we expect the action to vary quadratically with small variations about this path, so that closeby paths will all add coherently, whereas other paths will tend to interfere destructively.

To see how this works, consider a Lagrangian taking the form

$$\boxed{\mathcal{L} = \tfrac{1}{2}(m(t)\dot{Q}^2 - \Omega^2(t)Q^2) - F(t)Q} \tag{245}$$

ie., a particle with time-varying mass and time varying force acting on it, while sitting in a harmonic potential which is also time-varying.

Now we write the paths in the form

$$Q(t) = Q_c(t) + q(t) \tag{246}$$

where $Q_c(t)$ is the classical path, which satisfies the eqtn of motion

$$m(t)\ddot{Q}_c(t) + \Omega(t)Q_c(t) + F(t) = 0 \tag{247}$$

with boundary conditions $Q_c(t_1) = Q_1$, $Q_c(t_2) = Q_2$. Now if we expand the action around the classical minimum, as a functional of $q(t)$, we easily find that

$$S[Q] = S_c[Q_c] + \frac{1}{2}\frac{\delta^2 S'}{\delta Q^2}\bigg|_{Q=Q_c} q^2 + \dots \tag{248}$$

in symbolic form - the linear functional derivative is zero by assumption that $Q_c(t)$ is the path of minimum action. For the Lagrangian of (245), it follows immediately that we have

$$S[Q] = S_c[Q_c] + \int_{t_1}^{t_2} d\tau\, \tfrac{1}{2}[m(\tau)\dot{q}^2(\tau) - \Omega^2(\tau)q^2(\tau)] \tag{249}$$

with the boundary conditions

$$q(t_1) = q(t_2) = 0 \tag{250}$$

Now consider what form the propagator must take - we have

$$\boxed{G(Q_2, Q_2; t_1, t_2) = e^{\frac{i}{\hbar}S_c(1,2)} \int_{q(t_1)=0}^{q(t_2)=0} \mathcal{D}q(\tau)\, e^{\frac{i}{\hbar}S_{fl}[q]}} \tag{251}$$

where the "fluctuation" action here is

$$S_{fl}[q] = \int_{t_1}^{t_2} dt\, \tfrac{1}{2}[m(t)\dot{q}^2 + \Omega^2(t)q^2] \tag{252}$$

Note that $S_{fl}[q]$ is just the action for an oscillator (albeit with time-dependent mass and frequency) which starts and returns to the origin.

These results all suppose that we can ignore higher-order terms in (248), ie., terms in $\delta^n S/\delta Q^n$. The effect such terms might have will be discussed later in the course. Suppose we now stick to (251). We see that a computation of this involves 2 tasks, viz., (i) the calculation of the classical action, and (ii) the calculation of the Green function of the oscillator. We come to these tasks below.

Notice that the formula in (251) is quite general - it does not depend on the assumed action, ie, on the particular Lagrangian in (245). However it is often quite hard to find analytic answers to problems with more general Lagrangians, so for the moment we will stick to the special form in (245); for which (251) gives the exact answer.

Consider now the 2 stages involved in solving for (251), as follows:

(i) CLASSICAL ACTION : In principle the problem of finding the classical action is straightforward - we must solve either Lagrange's or Hamilton's eqtns for the system of interest, using the boundary conditions to fix the solution precisely. As the simplest possible example, consider the problem of a free particle, for which

$$L = \tfrac{1}{2} m \dot{x}^2 \qquad \text{(Free Particle)} \tag{253}$$

This problem is trivially solved; the general solution is: $x(t) = vt + c$ (254)
and with the boundary conditions $x(t_1) = x_1$, $x(t_2) = x_2$,
we have

$$x(t) = x_1 + \frac{x_2 - x_1}{t_2 - t_1} t \tag{255}$$

so that the classical action is

$$\left.\begin{aligned} S_c = \tfrac{1}{2} m \int_{t_1}^{t_2} dt\, \dot{x}^2 &= \tfrac{1}{2} m \frac{(x_2 - x_1)^2}{t_2 - t_1} \equiv \tfrac{1}{2} m v^2 (t_2 - t_1) \\ &\equiv E(t_2 - t_1) \equiv p(x_2 - x_1) \end{aligned}\right\} \tag{256}$$

where $E = \frac{1}{2} m v^2 = p^2/2m$. Thus the result can be thought of as sweeping out a region in phase space whose total area is the action, as we would expect from classical mechanics.

To find S_c for more complicated problems is not always so easy in practise, but poses no problems in principle provided a solution to the equations of motion exists.

(ii) FLUCTUATION DETERMINANT : The path integral over the fluctuations over the classical path is less straightforward. Note we can write it as

$$A(t_2, t_1) = \tilde{G}(0,0; t_2, t_1) \equiv \int_{q(t_1)=0}^{q(t_2)=0} \mathcal{D}q(\tau)\, e^{\frac{i}{\hbar} S_{fl}[q]} \tag{257}$$

where $\tilde{G}(q_2, q_1; t_2, t_1)$ is nothing but the Green's function for a system with Lagrangian

$$L_{fl}(q, \dot{q}; t) \equiv \tfrac{1}{2}[m(t)\dot{q}^2 - \Omega^2(t) q^2] \tag{258}$$

ie., $A(t_2, t_1)$ is just the "return amplitude" for a particle having the Lagrangian (258), after a time $t_2 - t_1$.

There are various ways to find this. Let's begin with the most direct way, which starts directly from the infinitesimal form of the path integral. This method is somewhat clumsy but it works; we therefore chop up the path for $q(\tau)$ into N pieces as before, and write the analogue of (224) as

$$A(t_2,t_1) = \lim_{\substack{N\to\infty \\ dt\to 0}} \prod_{j=1}^{N-1} \int dq_j\, \mathcal{A}_N \exp\left\{\frac{i}{\hbar} dt \sum_{j=1}^{N-1}\left[\frac{1}{2} m_j \left(\frac{q_{j+1}-q_j}{dt}\right)^2 - \frac{1}{2}\Omega_j^2 q_j^2\right]\right\} \qquad (259)$$

with $\mathcal{A}_N$ given by (225) as before, and $m_j = m(t_j = \frac{j}{N}(t_2-t_1)+t_1)$, etc. But notice that this result is just a quadratic form in the vector $\underline{\mathbf{q}} = (q_1, \ldots q_j \ldots q_{N-1})$, ie, we can write

$$A(t_2,t_1) = \mathcal{A}_N \prod_{j=1}^{N-1} \int dq_j \exp\{-\mathbf{q}\tilde{\mathbf{D}}\mathbf{q}\} \qquad (260)$$

where the exponential is shorthand for $\qquad \mathbf{q}\tilde{\mathbf{D}}\mathbf{q} \equiv \sum_{i,j=1}^{N-1} q_i \tilde{D}_{ij} q_j \qquad (261)$

and the matrix $\tilde{\mathbf{D}}$ is $\qquad \tilde{\mathbf{D}} = \hat{\mathbf{D}}_0 + \hat{\mathbf{D}}_1 \qquad (262)$

with the specific forms:

$$\tilde{\mathbf{D}}_0 = \frac{i}{2\hbar\, dt}\begin{pmatrix} 2m_1 & -1 & & 0 \\ -1 & 2m_2 & -1 & \\ & -1 & 2m_3 & \ddots \\ 0 & & -1 & \ddots \ddots \end{pmatrix} \qquad \tilde{\mathbf{D}}_1 = \frac{-i}{2\hbar}\Omega_j^2\, dt\, \boldsymbol{\delta}_{ij} \qquad (263)$$

ie., $\hat{\mathbf{D}}_0$ is a tridiagonal matrix which describes the kinetic part of the Lagrangian, and $\hat{\mathbf{D}}_1$ is a purely diagonal matrix which describes the interaction.

Now the advantage of writing $A(t_2,t_1)$ in this way is that we can then use the simple result that

$$\prod_{j=1}^{N-1}\int dq_j\, e^{-\mathbf{q}\tilde{\mathbf{D}}\mathbf{q}} = \left(\frac{\pi^{N-1}}{|\mathbf{D}|}\right)^{1/2} \qquad (264)$$

where $|\tilde{\mathbf{D}}| \equiv \det\tilde{\mathbf{D}}$ is the determinant of $\mathbf{D}$; this result is obvious if we diagonalise the quadratic form (which leaves the determinant invariant). Thus all we need to do is evaluate the determinant. Here I will give the general result without proof (the proof will appear in a supplementary appendix); but first let's see how it works with the simple case of a free particle.

For a free particle $\tilde{\mathbf{D}}_1 = 0$, and $\mathbf{D}_0$ takes the simple form

$$\hat{\mathbf{D}}_0 = \frac{1}{\hbar}\frac{m}{2dt}\begin{pmatrix} 2 & -1 & & 0 \\ -1 & 2 & -1 & \\ & -1 & 2 & \ddots \\ 0 & & \ddots & \ddots \end{pmatrix} \quad \text{(Free Particle)} \qquad (265)$$

and the determinant of this can be found by iteration, noting that

$$\left.\begin{aligned} d^0_{n+1} - 2d^0_n + d_{n-1} &= 0 \\ \text{and} \quad d^0_1 = 2 \qquad d^0_2 &= 3 \end{aligned}\right\} \qquad (266)$$

where $\frac{im}{2\hbar\, dt} d^0_n \equiv |\tilde{\mathbf{D}}_0|$, for an $n\times n$ matrix. One then easily finds: $\quad d^0_{N-1} = N \qquad (267)$

so that we have $\qquad |\tilde{\mathbf{D}}_0| = N\left(\frac{im}{2\hbar\, dt}\right)^{\frac{N-1}{2}} \qquad (268)$

It then immediately follows that

$$A(t_2,t_1) = \mathcal{A}_N \sqrt{\frac{\pi^{N-1}}{|\mathbf{D}_0|}} = \left(\frac{m}{2\pi i\hbar N dt}\right)^{1/2} \equiv \left(\frac{m}{2\pi i\hbar (t_2-t_1)}\right)^{1/2} \qquad (269)$$

so that we finally have the propagator

$$\boxed{G(x_2,x_1;t_2,t_1) = \left(\frac{m}{2\pi i\hbar (t_2-t_1)}\right)^{1/2} \exp\left\{\frac{i}{\hbar}\,\frac{m}{2}\,\frac{(x_2-x_1)^2}{t_2-t_1}\right\}} \quad \text{(FREE PARTICLE)} \qquad (270)$$

We will look at some features of this later. Let's first see how this result generalizes to more elaborate Lagrangians of the form given in (245). We must then deal with the determinant of the full matrix $\mathbf{D}$. Let us write this in the form

$$\tilde{\mathbf{D}} = \frac{i}{2\hbar\, dt}\tilde{\mathbf{\Delta}} \qquad (271)$$

where $\tilde{\mathbf{\Delta}}$ has the form

$$\begin{pmatrix} 2m_1 - \Omega_1^2 (dt)^2 & -1 & & \mathbf{0} \\ -1 & 2m_2 - \Omega_2^2 (dt)^2 & & \\ & -1 & \ddots & \\ \mathbf{0} & & & \ddots \end{pmatrix} \qquad (272)$$

Now we notice that the determinant $\Delta_n = |\mathbf{\Delta}|_{n\times n}$ satisfy the recursion relations

$$\Delta_{n+1} - \left(2 - \frac{\Omega_{j+1}^2}{m_{j+1}} (dt)^2\right)\Delta_n + \Delta_{n-1} = 0 \qquad (273)$$

which we can rewrite as

$$\frac{(\Delta_{n+1} - 2\Delta_n + \Delta_{n-1})}{(dt)^2} = \frac{\Omega^2}{m}\,\Delta_n \qquad (274)$$

However this is just the difference equation for a differential equation - if we let $t = t_1 + n\,dt$, and define the function $\phi(t,t_a) = \Delta(t)\,dt$, we have

$$\boxed{m(t)\,\ddot{\phi}(t,t_1) + \Omega^2 \phi(t,t_1) = 0} \qquad (275)$$

We can find the boundary conditions by noting that the first 2 values of Δ_n are

$$\Delta_0 = m_1 \qquad \Delta_1 = m_1\left(2 - \frac{\Omega_1^2}{m_1}(dt)^2\right) \qquad (276)$$

so that we have

$$\boxed{\begin{aligned} \phi(t_1,t_1) &= 0 \\ \dot{\phi}(t_1,t_1) &= 1 \end{aligned}} \qquad (277)$$

as initial value boundary conditions. Thus the determinant we want is the solution to (275) and (277) for $t \to t_2$, and our general solution is then

$$\boxed{G(x_2,x_1;t_2,t_1) = \left(\frac{1}{2\pi i\hbar\, \phi(t_2,t_1)}\right)^{1/2} \exp\left\{\frac{i}{\hbar} S_c(x_2,x_1;t_2,t_1)\right\}} \qquad (278)$$

Now anyone familiar with the theory of Green functions will realise that we have gone through a very lengthy derivation to get a result which could have been derived more simply. This is because a defining property of the Green function G which defines the prefactor in (257) is precisely that it satisfy the differential eqtn. (275), with the boundary conditions in (277). Thus we could have derived (278) in a more direct way. However I have not done so, simply because I wanted to make the link with the path integral formulation.

When we come to semiclassical theory we will see a more general formula than (278). However it is now useful to review some examples.

A.3.2.(b) <u>SOME EXAMPLES</u> : Here we will very briefly review the answers for a few examples, without giving derivations, but focussing more on their physical significance, and outlining a few of their main properties.

We have seen that the result for the propagator is given by the exponential of the classical action (time $i/\hbar$), multiplied by a <u>prefactor</u> $A(t_2,t_1)$ which is not exponential in form. We immediately see the link to the simple semiclassical ansatz introduced in (121), and it is interesting to see how this ansatz is filled out by real examples:

(1) <u>FREE PARTICLE</u> : We have already looked at the derivation here. The result easily generalizes to an arbitrary number of dimensions - in D dimensions one has

$$\boxed{G_D^0(\underline{r},t;0,0) = \left(\frac{m}{2\pi i\hbar t}\right)^{D/2} \exp\left\{\frac{i}{\hbar}\frac{m}{2}\frac{r^2}{t}\right\}} \qquad \text{(FREE PARTICLE)} \qquad (279)$$

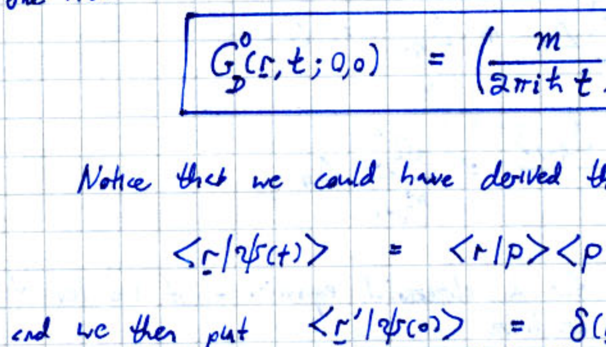
Notice that we could have derived this result directly with ease. If we start from

$$\langle \underline{r}|\psi(t)\rangle = \langle r|p\rangle\langle p|\hat{G}|p'\rangle\langle p'|r'\rangle\langle r'|\psi(0)\rangle \qquad (280)$$

and we then put $\langle \underline{r}'|\psi(0)\rangle = \delta(\underline{r}')$ (ie., the particle starts at the origin), and use $\langle p|G|p'\rangle = \delta_{pp'}\exp\{-i/\hbar \frac{p^2}{2m}t\}$, we immediately find that

$$G_0^{(0)}(r,t) = \sum_p e^{i/\hbar\,(p\cdot r - \frac{p^2}{2m}t)} \qquad (281)$$

which gives us back the same result as (279). It is interesting to look at the behaviour of this function. From (281) we see that the propagator superposes different planes waves that are weighted according to the factor $e^{i/\hbar\, p^2 t/2m}$ (which acts as a phase shift). The modulus of G is independent of $\underline{r}$ at any time, but what we have is a travelling wave with wavelength which shortens as we increase $|\underline{r}|$. This is simply because at a time t, any particle which reaches $\underline{r}$ must have velocity $v = r/t$, and so for large $|\underline{r}|$ it has high velocity and thus a short wavelength.



Re $G(r,t)$ [FREE PARTICLE]

(ii) <u>1-D HARMONIC OSCILLATOR</u> : We pick here a special case of the general Lagrangian in (245), where we now assume that

$$\mathcal{L} = \frac{m}{2}\left[\dot{x}^2 - \omega^2 x^2\right] \tag{282}$$

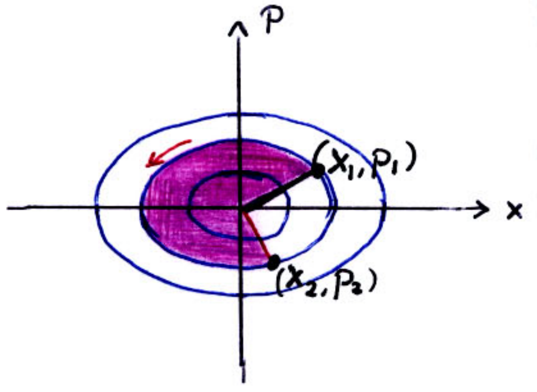
Although the result for the propagator depends only on the time difference $t = t_2 - t_1$, the answer must depend on x_2 and x_1 separately, since the potential is not invariant under translations. So we calculate

$$G(x_2, t; x_1, 0) = A(t)\, e^{i/\hbar\, S_c[x_2, x_1; t]} \tag{283}$$

where in fact

$$\boxed{\begin{aligned} A(t) &= e^{-i\pi/2\,[\omega t/\pi]} \left(\frac{m\omega}{2\pi\hbar\,|\sin\omega t|}\right)^{1/2} \\ S_c(x_2, x_1; t) &= \frac{m}{2}\frac{\omega}{\sin\omega t}\left[(x_1^2 + x_2^2)\cos\omega t - 2x_1 x_2\right] \end{aligned}} \tag{284}$$

Remarkably, the factor $e^{-i\pi/2\,[\omega t/\pi]}$, where $[x]$ denotes the largest integer less than x, was not found in this formula until 1975. It arises from "caustic" points in the dynamics of the system, and is not found in a derivation of the kind given above. We will return to this in the discussion of the semiclassical expansion. The rest of the fluctuation determinant prefactor is exactly what one expects from the general formula (278).



REGION IN PHASE SPACE SWEPT OUT BY OSCILLATOR BETWEEN t_1 AND t_2

Some understanding of the formula for the classical action is obtained by considering directly the integral for it - we have

$$\left.\begin{aligned} S_c &= \int_{t_1}^{t_2} dt\, L(x, \dot{x}) = \frac{m}{2}\int dt\left[\dot{x}^2 - \omega^2 x^2\right] \\ &\to \frac{m}{2}\left\{\left[x\dot{x}\right]_{t_1}^{t_2} - \int dt\, x(t)\left(\frac{d^2}{dt^2} + \omega^2\right)x(t)\right\} \\ &= \frac{m}{2}\left[x_2\dot{x}_2 - x_1\dot{x}_1\right] \end{aligned}\right\} \tag{285}$$

where we integrate by parts and use the eqtn of motion to throw away the 2nd term. We get exactly the same answer by considering the integral

$$S_c = \int_{x_1}^{x_2} p\, dx \tag{286}$$

which as we know measures the area swept out in phase space by the system between times t_1 and t_2. Now the soltn to the eqtn of motion is

$$x(t) = x_1 \cos\omega(t - t_1) + \frac{\dot{x}_1}{\omega}\sin\omega(t - t_1) \tag{287}$$

and direct substitution in (285) gives the classical action in (284).

(iii) <u>FREE PARTICLE ON A RING</u> : This is a very cute problem which we will find to be quite illuminating later on. The Lagrangian is written in the form

$$L = \tfrac{1}{2} I \dot{\theta}^2 \tag{288}$$

where I is the moment of inertia of the particle constrained to move on a ring of circular shape; if the radius of the ring is R then $I = mR^2$ for a particle of mass m.

Suppose we consider the Green function for this problem. We can immediately derive the answer from (279), if we notice that the amplitude for the particle to go from an angular coordinate θ_1 to θ_2 must sum over all possible winding numbers of the path - what we we mean is that the solution for $\theta_2 - \theta_1 = \theta$ is equivalent to paths on the line of length $\theta + 2n\pi$, where $n = -\infty, \dots \infty$. Thus we have

$$\boxed{\begin{aligned} G(\theta,t) &= \left(\frac{I}{2\pi i\hbar t}\right)^{1/2} \sum_{n=-\infty}^{\infty} \exp\left\{\frac{i}{\hbar} I \frac{(\theta+2n\pi)^2}{2t}\right\} \\ &\equiv \left(\frac{I}{2\pi i\hbar t}\right)^{1/2} \vartheta_3\left(\frac{\pi I\theta}{\hbar t}, \frac{2\pi I}{\hbar t}\right) e^{\frac{i}{\hbar} I\theta^2/2t} \end{aligned}} \tag{289}$$

where we use the Jacobi θ-function $\vartheta_3(z,t)$, defined as the series sum

$$\vartheta_3(z,t) = \sum_{n=-\infty}^{\infty} e^{i(2zn + \pi t n^2)} \tag{290}$$

whose properties we do not stop to examine here (it is a most remarkable function!). Thus all the effect of the topology of the system is to be found in this θ-function in the prefactor - otherwise $G(\theta,t)$ looks identical to the result (279) on a line.

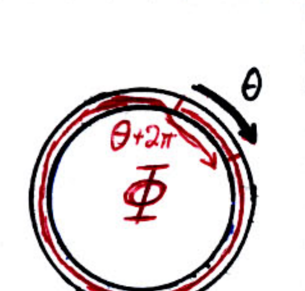
Note a curious feature of this problem. Suppose we add an extra topological phase in the ring - this can be done if the particle is charged by adding a flux through the ring, and the extra phase accumulated is then

$$\frac{e}{\hbar}\oint A.dl = 2\pi \frac{e}{h} \Phi = \Phi/\Phi_0 = \phi \tag{291}$$

where $\Phi = h/e$ is the flux quantum, and Φ is the flux through the ring.

Now, quite dramatically, we see that different winding numbers are distinguished by having different phases accumulated - a path with winding number n accumulates an extra "topological flux phase" of $n\phi$.

The resulting propagator is



PROPAGATION ROUND A RING WITH ENCLOSED FLUX Φ; AN PHASE ϕ IS ADDED ON EACH EXTRA CIRCUIT.

$$\boxed{\begin{aligned} G(\theta;\phi;t) &= \left(\frac{I}{2\pi i\hbar t}\right)^{1/2} \sum_n \exp\left\{in\phi + \frac{i}{\hbar} I \frac{(\theta+2n\pi)^2}{2t}\right\} \\ &\equiv \left(\frac{I}{2\pi i\hbar t}\right)^{1/2} \vartheta_3\left(\frac{\pi I\theta}{\hbar t} - \frac{\phi}{2}; \frac{2\pi I}{\hbar t}\right) e^{\frac{i}{\hbar} I\theta^2/2t} \end{aligned}} \tag{292}$$

Note that, as we would expect, this result is completely periodic in ϕ; increasing ϕ by 2π makes no difference to the answer.

One can also get these answers by simply solving the Schrodinger eqtn on the ring, and using the form (213) for $G(\theta,t)$, ie

$$G(\theta,t) = \sum_l \psi_l(\theta)\psi_l^*(0)\, e^{i/\hbar\, E_l t} \tag{293}$$

where

$$\psi_l(\theta) = \frac{1}{\sqrt{2\pi}} \exp\{i(l + \phi/2\pi)\theta\} \tag{294}$$

and where the eigenenergies are

$$\epsilon_l = \frac{\hbar^2}{2I}\left(l + \phi/_{2\pi}\right)^2 \tag{295}$$

and the quantity $L = \hbar l$ has the meaning of angular momentum ; l is an integer. Notice that the flux thus also changes the energy of all the states, but this change is not periodic (as we would expect - we are increasing the effective angular momentum by increasing ϕ). However $G(\theta, t)$ is still periodic since it depends only on the phase accumulated in a circuit as the exponent of $i \times$(this phase).

(iv) A TWO-LEVEL SYSTEM : At first glance one should not be able to compute the propagator for a TLS using path integral theory because it has no classical analogue. However we note that (i) we can easily get a result for $\hat{G}$ without ever using path integrals; and (ii) we will see that we can easily re-interpret this answer as a sum over a certain set of paths.

Let us consider the problem described by a Hamiltonian

$$\mathcal{H}_0^{TLS} = \hbar\left(\Delta_0 \hat{\tau}_x + \epsilon_0 \hat{\tau}_z\right) \tag{296}$$

where Δ and ϵ are in frequency units. Note that we do not have as yet a Lagrangian for this system, or for the spin-½ system it corresponds to.

Nevertheless, if we define eigenstates $|\uparrow\rangle, |\downarrow\rangle$ of the operator $\hat{\tau}_z$, labelling these states as $|\tau_z\rangle$, we can derive an expression for the propagator $G(\tau_z, \tau_z'; t, t')$ using ordinary operator methods, in a direct calculation of

$$G(\tau_z, \tau_z'; t, t') = \langle \tau_z | e^{-i/\hbar H_0^{TLS} t} | \tau_z' \rangle \tag{297}$$

by simply expanding the exponential.

Symmetric Case : Let us first choose $\epsilon_0 = 0$, ie., we have a spin-½ in a transverse field (which classically would simply precess around this field). The QM result is just

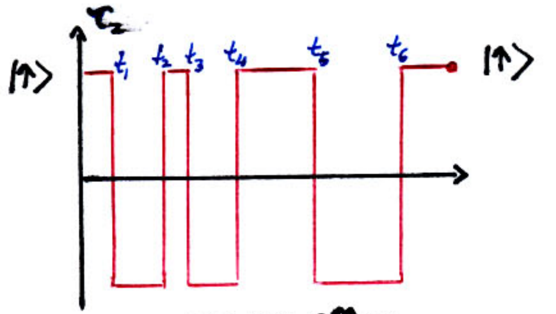
$$\left.\begin{aligned} G_0(\tau_z, \tau_z'; t) &= \langle \tau_z | e^{-i\Delta_0 \hat{\tau}_x t} | \tau_z' \rangle \\ &= \langle \tau_z | \cos\Delta_0 t - i\hat{\tau}_x \sin\Delta_0 t | \tau_z' \rangle \\ &= \delta_{\tau_z \tau_z'} \cos\Delta_0 t - i\,\delta_{\tau_z, -\tau_z'} \sin\Delta_0 t \end{aligned}\right\} \tag{298}$$

ie, we have

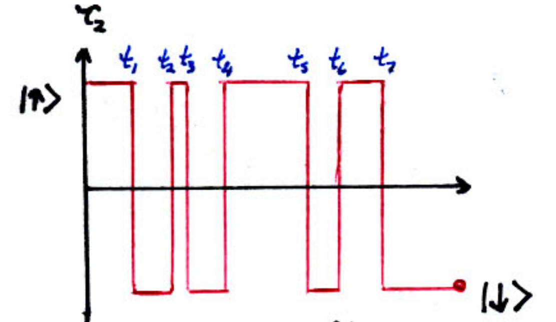
$$\left.\begin{aligned} G_0^{\uparrow\uparrow}(t) &= G_0^{\downarrow\downarrow}(t) = \cos\Delta_0 t \\ G_0^{\uparrow\downarrow}(t) &= G_0^{\downarrow\uparrow}(t) = -i\sin\Delta_0 t \end{aligned}\right\} \tag{299}$$

But now suppose we re-interpret the exponential as follows. Expand the exponential as

$$\left.\begin{aligned} e^{-i\Delta_0 \hat{\tau}_x t} &= 1 + \sum_{n=1}^{\infty} \frac{(-i\Delta_0 t)}{n!}\hat{\tau}_x^{\,n} \\ &= \sum_{n=0}^{\infty}\left\{ \frac{(-i\Delta_0 t)^{2n}}{(2n)!} + \frac{(-i\Delta_0 t)^{2n+1}}{(2n+1)!}\hat{\tau}_x \right\} \end{aligned}\right\} \tag{300}$$



PATH FOR $G_0^{\uparrow\uparrow}(t)$



PATH FOR $G_0^{\uparrow\downarrow}(t)$

and now let's write these sums as

$$\left.\begin{aligned} \cos\Delta_0 t &= \sum_{n=0}^{\infty}(-i\Delta_0)^{2n}\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1 \\ \sin\Delta_0 t &= \sum_{n=0}^{\infty}(-i\Delta_0)^{2n+1}\int_0^t dt_{2n+1}\int_0^{t_{2n+1}}dt_{2n}\cdots\int_0^{t_2}dt_1 \end{aligned}\right\} \quad (301)$$

But this shows we can reinterpret the summation in (300) as follows. Assign a path to τ_z, such that the $|\uparrow\rangle, |\downarrow\rangle$ states correspond to ± 1 values; and assign a factor

$$\Delta S = -i\Delta_0\, dt\ \delta(t-t_j) \qquad (302)$$

for the contribution to S from a flip at $t=t_j$. Now allow these spin flips to occur at random along the time axis, with some arbitrary number n of them - then sum over all n, and integrate over all possible times for the flips. The only restriction is that $G_0^{\uparrow\uparrow}$ involve an even number of flips, and $G_0^{\uparrow\downarrow}$ involves an odd number. Typical paths are shown at left.

<u>Asymmetric Case</u>: This is a little more complicated because the Hamiltonian is now acting in between the flips (as well as just during the flips, as happens for the symmetric case). From the argument given above, we might now expect a contribution

$$\Delta S = i\epsilon_0 \tau_z\, dt \qquad (303)$$

to the action. Notice that (i) there is no delta-fn of time - this term acts at all times between flips; (ii) its sign depends on the orientation of τ_z (iii) its magnitude is ϵ_0. All this can be guessed just by looking at (294) and letting $t \to dt$.

What we are saying, in effect, is that we can make the following expansions:

$$\boxed{\begin{aligned} G_0^{\uparrow\uparrow}(t) &= \langle\uparrow| e^{-i(\Delta_0\hat{\tau}_x+\epsilon_0\hat{\tau}_z)t}|\uparrow\rangle = \sum_{n=0}^{\infty}(-i\Delta_0)^{2n}\int_0^t dt_{2n}\, e^{i\epsilon_0(t-t_{2n})}\int_0^{t_{2n}}dt_{2n-1}\, e^{-i\epsilon_0(t_{2n}-t_{2n-1})}\cdots \\ G_0^{\uparrow\downarrow}(t) &= \langle\uparrow| e^{-i(\Delta_0\hat{\tau}_x+\epsilon_0\hat{\tau}_z)t}|\downarrow\rangle = \sum_{n=0}^{\infty}(-i\Delta_0)^{2n+1}\int_0^t dt_{2n+1}\, e^{-i\epsilon_0(t-t_{2n+1})}\int_0^{}dt_{2n}\, e^{i\epsilon_0(t_{2n+1}-t_{2n})}\cdots \end{aligned}} \quad (304)$$

as can be verified by detailed inspection. To evaluate these integrals, it is easy to simply Laplace transform them, ie write

$$G_0^{\alpha\beta}(t) = \int_{-i\infty}^{i\infty} e^{pt}\, G_0^{\alpha\beta}(p) \qquad (305)$$

so that, eg.,

$$G_0^{\uparrow\uparrow}(p) = \frac{1}{p-i\epsilon_0}\sum_{n=0}^{\infty}\frac{(-i\Delta_0)^{2n}}{(p^2+\epsilon_0^2)^n} \equiv \frac{1}{p-i\epsilon_0}\,\frac{p^2+\epsilon_0^2}{p^2+E_0^2} \qquad (306)$$

where the ~~total~~ splitting energy is

$$\hbar E_0 = \hbar(\epsilon_0^2+\Delta_0^2)^{1/2} \qquad (307)$$

Doing the inverse Laplace transform of (306) immediately yields

$$G_0^{\uparrow\uparrow}(t) = \cos E_0 t + i\frac{\epsilon_0}{E_0}\sin E_0 t \qquad (308)$$

and one can do a similar analysis for $G_0^{\uparrow\downarrow}(t)$, etc.

The reason of course why we have been able to do this problem, even though we do not have a classical analogue for the TLS, is that the problem is so simple that we can simply expand the exponential in a power series in the fundamental expressions (304), because we can do a sensible discretisation of the path. In effect the Trotter product has turned into a much simpler product.

(v) <u>A DRIVEN HARMONIC OSCILLATOR</u>: Finally, in this list of problems let us consider a more complicated problem, which is still in the general class of problems defined by the Lagrangian (245), with its solution in (278). The novel feature of this Lagrangian is its time-dependence - we have an external driving force:

$$\mathcal{L} = \tfrac{1}{2}m(\dot{x}^2 - \omega_0^2 x^2) - F(t)\,x(t) \qquad (309)$$

Let us remark immediately that the key physical difference here is that $\mathcal{L}(t)$, because it is time-dependent, must be describing an open system. The key mathematical difference is that everything now depends on the arbitrary function $F(t)$; so all physical quantities, and also the propagator, now become <u>functionals</u> of $F(t)$.

From the discussion leading to (278), we know that the form (278) actually gives the exact answer for this problem - thus it remains only to evaluate the classical action, & the fluctuation determinant, which we do in turn:-

<u>Classical Action</u>: This is actually the most complicated part of the job - we have to find an appropriate expression for the solution to the equation of motion, so that can be integrated up to get the action.

The eqtn of motion is

$$m(\ddot{x} + \omega_0^2 x) = -F(t) \qquad (310)$$

and this can be solved for $x(t)$ in various ways. For example, we can write it in the form of the sum of the soltn to the homogeneous eqtn (where $F(t)=0$) plus a particular soltn to the inhomogeneous eqtn; we write this as

$$x(t) = \left(A\cos\omega_0 t + B\sin\omega_0 t\right) - \frac{1}{m\omega_0}\int_{t_1}^{t} dt'\,F(t')\sin\omega_0(t'-t_1) \qquad (311)$$

where A and B remain to be fixed by the boundary conditions - the form chosen for the particular solution is that we would get by assuming that $x(t_1)$ and $\dot{x}(t_1)$ are zero.

The boundary conditions are of course

$$\left.\begin{aligned} x(t_1) &= x_1 \\ x(t_2) &= x_2 \end{aligned}\right\} \qquad (312)$$

and we want to find $G(x_2 x_1; t_2, t_1 \mid F(t))$. From the boundary conditions we can fix A and B; we find

$$\left.\begin{aligned} A &= x_1 \\ B &= \frac{1}{\sin\omega_0(t_2-t_1)}\left\{\left[x_2 - x_1\cos\omega_0(t_2-t_1)\right] + \frac{1}{m\omega_0}\int_{t_1}^{t_2} dt'\,F(t')\sin\omega_0(t_2-t')\right\} \end{aligned}\right\} \qquad (313)$$

Now let's consider how to calculate the action. We use the same trick as with the unperturbed oscillator, i.e., calculate the area swept out in phase space by the system. However now we have

$$\left.\begin{aligned} S_c(2,1) &= \int_{t_1}^{t_2} dt \left\{ \tfrac{1}{2}m(\dot{x}^2 - \omega_0^2 x^2) - F(t)x \right\} \\ &= \tfrac{1}{2}m\left[\dot{x}x\right]_{t_1}^{t_2} - \tfrac{1}{2}\int d\tau \left\{ x(\tau)\left(m\frac{d^2}{d\tau^2} + m\omega_0^2\right)x(\tau) + F(\tau)x(\tau) \right\} \\ &= \frac{m}{2}\left[x_2\dot{x}_2 - x_1\dot{x}_1\right] - \tfrac{1}{2}\int_{t_1}^{t_2} d\tau\, F(\tau)x(\tau) \end{aligned}\right\} \quad (314)$$

where as before we integrate by parts, and notice this time that

$$m\int d\tau\, x(\tau)\left[\frac{d^2}{d\tau^2} + \omega_0^2\right]x(\tau) \equiv -\int d\tau\, F(\tau)x(\tau) \quad (315)$$

from the eqtn of motion. We now substitute the solution ((311) and (313)) for $x(t)$ into the result (314) for S_c, and after considerable manipulations, none of which are difficult, we get the answer in the form

$$\boxed{S_c(2,1) = S_c^0(2,1) + S_c^F(2,1)} \quad (316)$$

where

$$S_c^0(2,1) = \frac{m}{2}\frac{\omega_0}{\sin\omega_0(t_2-t_1)}\left\{(x_1^2+x_2^2)\cos\omega_0(t_2-t_1) - 2x_1x_2\right\} \quad (317)$$

and

$$\boxed{\begin{aligned} S_c^F(2,1) = -\frac{1}{\sin\omega_0(t_2-t_1)}\Big\{ &\int_{t_1}^{t_2} d\tau\, F(\tau)\left[x_1\sin\omega_0(t_2-\tau) + x_2\sin\omega_0(\tau-t_1)\right] \\ &+ \frac{1}{m\omega_0}\int_{t_1}^{t_2} d\tau \int_{t_1}^{\tau} d\tau'\, F(\tau)F(\tau')\sin\omega_0(t_2-\tau)\sin\omega_0(\tau'-t_1)\Big\} \end{aligned}} \quad (318)$$

where the "bare" term S_c^0 is just that for the free oscillator (cf eqtn (284)), and the other term is the addition caused by the arbitrary force. Eqtn (318) is exact.

Fluctuational Prefactor: This is actually given by exactly the same form as the bare oscillator – that is, by (284). This is because adding a term linear in $x(\tau)$ cannot change the calculation of $A(t)$ in (269) [the eqtn of motion (275) is unaltered].

Thus the final result for the propagator is

$$\boxed{G(x_2,x_1;t_2,t_1|F) = A^0(t_2-t_1)\, e^{i/\hbar\, S_c(2,1;[F])}} \quad (319)$$

with $A^0(t_2-t_1)$ given by (284), and $S_c(2,1;[F])$ given by (316)-(318).

This concludes the intro to path integrals. The main thing to be emphasized is that they give exact answers for Lagrangians that can be written as quadratic forms (eg., like (248)) in the coordinates. However we have left out many things – these include:

- Other interesting examples of quadratic Lagrangians; eg., a parametric oscillator (where the frequency is time-dependent), with or without a driving force; or a charged particle coupled to an EM field (which gives couplings $\propto x\dot{x}$).

- Non-quadratic Lagrangians, with more complex potentials.

- Spins, and other quantum systems with a discrete spectrum.