PATH INTEGRALS AND INSTANTONS

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1 Path Integrals in Quantum Mechanics

A mechanical system in d-dimensions is described a a set of coordinates $\mathbf{q} \equiv \{q_1, q_2 \cdots q_d\}$[1] and their momenta $\dot{\mathbf{q}} \equiv \{\dot{q}_1, \dot{q}_2 \cdots \dot{q}_d\}$, and a Lagrangian $L[\mathbf{q}(t), \dot{\mathbf{q}}(t)]$, which is a functional of the coordinates and velocities.

Associated with each coordinate is a canonical momentum

$$p_i(t) \;=\; \frac{\delta L}{\delta \dot{q}_i}. \tag{1.1}$$

This enables us to define the kinetic energy,T, and potential energy, V, of the system

$$\begin{aligned} L = \;& T - V \\ T \quad = \quad & \frac{1}{2}\sum_{i=1}^{d} p_i \dot{q}_i \end{aligned} \tag{1.2}$$

If the system coordinates are functions of time, $\mathbf{q}(t)$, with initial values $\mathbf{q}(t_i) = \mathbf{q}_i$ and final values $\mathbf{q}(t_f) = \mathbf{q}_f$ then those functions are called a "path", between those initial and final values and we can define an "action", $S[\mathbf{q}(t)]$, which is a functional of the path by

$$S[\mathbf{q}(t)] \;\equiv\; \int_{t_i}^{t_f} L(\mathbf{q}(t), \dot{\mathbf{q}}(t))dt \tag{1.3}$$

The Lagrange equations of motion are derived from the postulate that the path between given initial and final conditions is the path for which the action is minimal.

The fundamental equation of Quantum Mechanics in terms of such an action can be written

$$\langle \mathbf{q}_f, t_f \big| \mathbf{q}_i, t_i \rangle \;=\; \int \mathcal{D}[\mathbf{q}(t)] \exp\left(i \frac{S[\mathbf{q}(t)]}{\hbar} \right), \tag{1.4}$$

[1] d is the total number of time-dependent coordinates required to specify the system - not the literal number of dimensions of the space in which the system is embedded, e.g for a two-particle system moving in three dimension's, $d = 6$.

where $\langle \mathbf{q}_f, t_f \big| \mathbf{q}_i, t_i \rangle$ is the quantum time-evolution amplitude for the system to propagate in time between a state at initial time t_i in which the coordinates take the values $\mathbf{q}_i$ to a state at final time t_f in which the coordinates take the values $\mathbf{q}_f$. The integral on the RHS of (1.4) is over *all* possible paths, $\mathbf{q}(t)$ with initial values $\mathbf{q}(t_i) = \mathbf{q}_i$ and final values $\mathbf{q}(t_f) = \mathbf{q}_f$. A definition of the integration measure $\mathcal{D}[\mathbf{q}(t)]$ will be discussed when we consider some explicit examples.

For a classical (macroscopic) system)the only path that will contribute to the path integral will be the path corresponding to an extremum of the action, since other paths whose action differs from the extremal action by an amount much larger than $\hbar$ will give rise to very rapid oscillations which will cancel out. But for microscopic systems we need to sum over all paths which differ from the classical path by an amount which is of the order of $\hbar$. Thus to calculate the quantum amplitude (and subsequently the probability) for a particle to be at $\mathbf{q}_f$ at time $t = t_f$, requires a weighted "sum over all histories" from an initial condition $\mathbf{q}_i$ at time $t = t_i$. This is a generalisation of the interpretation of the double slit experiment, in which the amplitude for a photon to land at a particular place on a screen os the sum over the amplitude for the photon to pass through one slit *and* the amplitude for the photon to pass through the other slit.

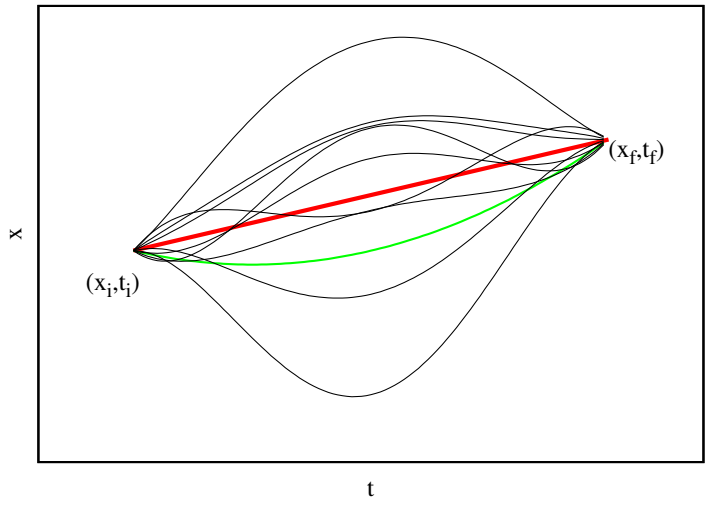

Figure 1: Some of the paths for a free particle moving between (x_i, t_i) and (x_f, t_f). The ticker red straight line is the classical path which obeys Newtons laws of motion.

An illustration of some of the paths which need to be taken into account is shown in Fig.1 , which considers the paths of a free particle moving in one dimension with coordinate x. From Newton's first law the particle moves in a straight line with constant velocity, indicated by the thicker red line between the initial and final positions. But for a quantum amplitude we need to sum over all possible paths, some of which are shown in the figure, notwithstanding the fact that a free classical free particle does not move along such paths.

In the case under consideration (a free particle with mass m), the classical path is given by

$$x(t) = x_i + \frac{(t-t_i)}{(t_f-t_i)}(x_f - x_i) \tag{1.5}$$

and the corresponding action is

$$S_{cl} \;=\; \frac{m}{2(t_f-t_i)}(x_f-x_i)^2. \tag{1.6}$$

But let us consider a different path, given by

$$x'(t) = x_i + \left(\frac{(t-t_i)}{(t_f-t_i)} + 2\frac{(t-t_i)(t-t_f)}{(t_f-t_i)^2}\right)(x_f - x_i), \tag{1.7}$$

which also satisfies the boundary values $x(t_i) = x_i,\ x(t_f) = x_f$. This path is shown as the green line in Fig.1. The action for this path is

$$S[x'(t)] \;=\; \frac{5m}{6(t_f-t_i)}(x_f-x_i)^2. \tag{1.8}$$

If m is of the order of the electron mass ($\sim 10^{-30}$kg.), $(x_f - x_i)$ is of the order of an atomic radius ($\sim 10^{-10}$m.), and $(t_f - t_i)$ is of the order of the period of oscillation of light ($\sim 10^{-15}$s.), then the difference between the action for the two paths is of order of $\hbar$ and so the path x' contributes to the transition amplitude almost as much as the classical action.

2 Relation between Path Integral and Schroedinger Equation

In this section we show the equivalence of the path integral expression (1.4) and the Schroedinger approach, which (in its time-integrated form) gives the quantum amplitude for a particle in a state $\big|k\rangle$ at time t_i to propagate in time to a state $\big|l\rangle$ at time t_f.

Using the integrated form of the Schroedinger equation this amplitude is

$$\langle l, t_f \big| k, t_i > = \;\langle l \left| \exp\left\{-i/\hbar \int_{t_i}^{t_f} \hat{H} dt\right\}\right| k\rangle \tag{2.1}$$

Inserting complete sets of eigenstates of $\hat{\mathbf{q}}(t)$,

$$\int d^d\mathbf{q}\, |\mathbf{q}\rangle\langle\mathbf{q}| \;\; = 1,$$

between initial and final states, this becomes

$$\langle l, t_f \big| k, t_i > = \int d^d\mathbf{q}_f d^d\mathbf{q}_i \Psi_l^*(\mathbf{q}_f)\langle \mathbf{q}_f \left| \exp\left\{-i/\hbar \int_{t_i}^{t_f} \hat{H} dt\right\}\right| \mathbf{q}_i\rangle \Psi_k(\mathbf{q}_i), \tag{2.2}$$

where

$$\Psi_k(\mathbf{q}) \;\equiv\; \langle \mathbf{q} \big| k \rangle$$

is the (time-independent) wavefunction for a system in state $\big|k\rangle$ (and similarly $\Psi_l(\mathbf{q})$). Eq.(2.2) can be rewritten

$$\langle \mathbf{q}_f, t_f \big| \mathbf{q}_i, t_i \rangle \;=\; \langle \mathbf{q}_f \left| \exp\left\{ -\frac{i}{\hbar} \int_{t_i}^{t_f} \hat{H} dt \right\} \right| \mathbf{q}_i \rangle \tag{2.3}$$

The time interval $(t_f - t_i)$ can be divided into a large number of intervals, N,

and at each time-slice, t_r, we insert unity in the form of a complete set of eigenstates of the coordinates

$$1 \;=\; \int d^d\mathbf{q}_r \big| \mathbf{q}_r \rangle\langle \mathbf{q}_f \left| \exp\left\{ -i/\hbar \int_{t_i}^{t_f} \hat{H} dt \right\} \right| \mathbf{q}_i \rangle\langle \mathbf{q}_r \big|.$$

Eq.(2.3) then becomes

$$\langle \mathbf{q}_f, t_f \big| \mathbf{q}_i, t_i \rangle \;=\; \lim_{N\to\infty} \prod_{r=0}^{N} \left\{ \int d^d\mathbf{q}_r \langle \mathbf{q}_{r+1} \left| \exp\left(-\frac{i}{\hbar} \hat{H} \Delta t \right) \right| \mathbf{q}_r \rangle \right\} \delta^d\left(\mathbf{q}(t_f) - \mathbf{q}_f\right) \delta^d\left(\mathbf{q}(t_i) - \mathbf{q}_i\right) \tag{2.4}$$

with $\Delta t \equiv (t_f - t_i)/N$ and the δ-functions ensure that the values of the coordinates are fixed at times t_i and t_f.

By inserting unity again, but this time as a complete set of eigenstates of the canonical momenta, $\mathbf{p}_r$, we can write the Hamiltonian operator $\hat{H}$ as a function of the canonical momenta and coordinates, so that we have

$$\langle \mathbf{q}_{r+1} \left| \exp\left\{ -\frac{i}{\hbar} \hat{H} \Delta t \right\} \right| \mathbf{q}_r \rangle \;=\; \int d^d\mathbf{p}_r \langle \mathbf{q}_{r+1} \left| \exp\left\{ -\frac{i}{\hbar} H(\mathbf{p}_r, \mathbf{q}_r) \Delta t \right\} \right| \mathbf{p}_r \rangle \frac{1}{(2\pi\hbar)^{d/2}} \exp\left\{ \frac{i}{\hbar} \mathbf{p}_r \cdot \mathbf{q}_r \right\}, \tag{2.5}$$

where we have used

$$\langle \mathbf{p} \big| \mathbf{q} \rangle \;=\; \frac{1}{(2\pi\hbar)^{d/2}} \exp\left\{ \frac{i}{\hbar} \mathbf{p} \cdot \mathbf{q} \right\}. \tag{2.6}$$

The factor involving the Hamiltonian is just a multiplicative constant since the Hamiltonian is a function of coordinates and momenta (as opposed to an operator) so we may take this outside $\langle \mathbf{q}_{(r+1)} \big|$ and again using Eq.(2.6) we have

$$\langle \mathbf{q}_{r+1} \left| \exp\left\{ -\frac{i}{\hbar} \hat{H} \Delta t \right\} \right| \mathbf{q}_r \rangle \;=\; \int d^d\mathbf{p}_r \exp\left\{ -\frac{i}{\hbar} H(\mathbf{p}_r, \mathbf{q}_r) \Delta t \right\} \frac{1}{(2\pi\hbar)^d} \exp\left\{ \frac{i}{\hbar} \mathbf{p}_r \cdot \left(\mathbf{q}_r - \mathbf{q}_{(r+1)} \right) \right\}, \tag{2.7}$$

Over a small time interval, Δt, we have

$$\left(\mathbf{q}_{(r+1)} - \mathbf{q}_r \right) \approx \dot{\mathbf{q}}_r \Delta t$$

Now we assume that the Hamiltonian is a quadratic function of the momenta

$$H(\mathbf{p}, \mathbf{q}) \;=\; \frac{1}{2} \mathbf{p}^T \cdot \mathbf{M}^{-1} \cdot \mathbf{p} + V(\mathbf{q}), \tag{2.8}$$

where M is the mass matrix[2] The integral over the momenta $\mathbf{p}_r$ is now a gaussian integral, which may be performed to yield

$$\begin{aligned}\langle \mathbf{q}_{r+1} \left| \exp\left\{ -\frac{i}{\hbar}\hat{H}\Delta t \right\} \right| \mathbf{q}_r \rangle &= \left(-\frac{i}{\hbar}\frac{\det \mathbf{M}}{2\pi\hbar\Delta t} \right)^{1/2} \exp\left\{ \frac{i}{\hbar}\left(\frac{1}{2}\dot{\mathbf{q}}_\mathbf{r}^T \cdot \mathbf{M} \cdot \dot{\mathbf{q}}_\mathbf{r} - V(\mathbf{q}_r) \right) \Delta t \right\} \\ &= \left(-\frac{i}{\hbar}\frac{\det \mathbf{M}}{2\pi\Delta t} \right)^{1/2} \exp\left\{ \frac{i}{\hbar} L(\mathbf{q}_r, \dot{\mathbf{q}}_r)\Delta t \right\} \end{aligned} \tag{2.9}$$

Inserting this back into Eq.(2.4), we see that we recover Eq.(1.4), provided we identify the measure for the integral over all paths by

$$\mathcal{D}[\mathbf{q}(t)] \equiv \lim_{N\to\infty} \prod_{r=1}^{N-1} \left(-i\frac{N \det \mathbf{M}}{2\pi\hbar\,(t_f - t_i)} \right)^{1/2} d^d\mathbf{q}(t_r) \tag{2.10}$$

Note that the values of the index r in the product goes over $r = 1$ to $r = (N-1)$, because the end-point values of $\mathbf{q}$ at $t = t_i,\ (r = 0)$ and $t = t_f, (r = N)$ are fixed.

The integration over all values of $\mathbf{q}$ at each time-slice between t_i and t_f makes perfect sense, since there will be at least one path for which at time t_r the coordinates $\mathbf{q}$ will take any given set of values, so that a sum over all paths must include all values. The pre-factor is required in the definition of the measure in order to link the path integral expression for the time evolution of a given state with that given by the Schroedinger equation.

The expression (2.10) is indeed very cumbersome, but we will see in the next section that there is an alternative way to express the measure, which is much more manageable.

3 Examples

3.1 Example 1: Free Particle

We consider a free particle of mass m moving (non-relativistic ally) in one dimension, with coordinate $x(t)$.

The Lagrangian is given by

$$L = \frac{1}{2}m\dot{x(t)}^2 \tag{3.1}$$

and the action is

$$S[x(t)] = \int_{t_i}^{t_f} \frac{1}{2}m\dot{x(t)}^2 dt \tag{3.2}$$

The classical solution which passes through the point x_i at time t_i and t_f at time t_f is

$$x_{cl}(t) = x_i + \frac{X}{T}(t - t_i), \tag{3.3}$$

[2]This matrix could also depend on the coordinates $\mathbf{q}$, for example in the case of particles moving in the presence of a gravitational with a non-Minkowski metric.

with $T \equiv t_f - t_i$ and $X \equiv x_f - x_i$ giving rise to a classical action

$$S_{cl} \;=\; \frac{m}{2}\frac{X^2}{T} \tag{3.4}$$

Now let us write the path $x(t)$ as the classical path, $x_{cl}(t)$ plus a quantum correction, $x_{qu}(t)$:

$$x(t) = x_{cl}(t) + x_{qu}(t) \tag{3.5}$$

and the quantum correction may be expanded as

$$x_{qu}(t) \;=\; \sum_{n=1}^{\infty} c_n \phi_n(t), \tag{3.6}$$

where $\phi_n(t)$ are a complete set of orthonormal functions. It is convenient to take these eigenfunctions to be the eigenfunctions of the operator $\hat{\mathcal{O}}$, where the action is written

$$S[x(t)] \;=\; S_{cl} + 2\pi\hbar \int_{t_i}^{t_f} dt \sum_{l,n} c_l^* c_n \phi_l^*(t) \hat{\mathcal{O}} \phi_n(t) \tag{3.7}$$

After integration by parts we see that the operator $\hat{\mathcal{O}}$ is

$$\hat{\mathcal{O}} \;= -\frac{m}{2}\frac{d^2}{dt^2} \tag{3.8}$$

Since all paths have to path through x_i at t_i and x_f at t_f, the eigenfunctions ϕ_n must vanish at $t = t_i$ and $t = t_f$. The eigenfunctions of $\hat{\mathcal{O}}$ which obey these boundary values are

$$\phi_n(t) \;=\; \sqrt{\frac{1}{T}} \sin\left(\frac{n\pi(t - t_i)}{T}\right) \tag{3.9}$$

These are orthonormal functions and so

$$\int_{t_i}^{t_f} dt \phi_l^*(t) \hat{\mathcal{O}} \phi_n(t) \;=\; \frac{m\pi^2}{2T^2} n^2 \delta_{ln}$$

The eigenvalues, λ_n are given by

$$\lambda_n = \frac{m n^2 \pi^2}{2T^2}$$

The action arising from a path whose coefficients[3] are c_n, is

$$S(\{c_n\} \;=\; S_{cl} + \sum_n c_n^2 \frac{m\pi^2}{2T^2} n^2 \tag{3.10}$$

[3]In this case the coefficients may be considered to be real, but in general we need to allow for these to be complex.

Integrating over all paths is equivalent to integrating over all values of the coefficients c_n, up to some jacobian, J, which we fix by comparing the result with that obtained from the Schroedinger approach.[4]

Therefore for a free particle we obtain

$$\langle x_f, t_f | x_i, t_i \rangle \;=\; \exp\left(i\frac{S_{cl}}{\hbar}\right) \det J \prod_{n=1}^{\infty} \int dc_n \exp\left\{ i\left(\frac{m\pi^2}{2\hbar T}\right) n^2 c_n^2 \right\}, \tag{3.11}$$

with $T = (t_f - t_i)$ The gaussian integrals over c_n can be performed yielding

$$\langle x_f, t_f | x_i, t_i \rangle \;=\; \exp\left(i\frac{S_{cl}}{\hbar}\right) \det J \prod_{n=1}^{\infty} \sqrt{\frac{-i\hbar T}{\pi m}} \frac{2}{n}. \tag{3.12}$$

with S_{cl} given by (3.4).

In the Schroedinger approach in the case of a free particle, the momentum eigenfunctions are also eigenfunctions of the Hamiltonian, $H = p^2/2m$, and so we have

$$\begin{aligned}
\langle x_f, t_f | x_i, t_i \rangle &= \frac{1}{2\pi\hbar} \int dp dp' \exp\left\{ \frac{i}{\hbar}\left(p' x_f - p x_i\right) \right\} \langle p' | \exp\left\{ i\frac{\hat{p}^2 T}{(2m\hbar)} \right\} | p \rangle \\
&= \frac{1}{2\pi\hbar} \int dp dp' \exp\left\{ i\frac{(p' t_f - p t_i)}{\hbar} \right\} \exp\left\{ i\frac{p^2 T}{2m\hbar} \right\} \delta(p - p') \\
&= \frac{1}{2\pi\hbar} \int dp \exp\left\{ i\frac{(pX - p^2 T)}{(2m\hbar)} \right\}
\end{aligned} \tag{3.13}$$

Performing the gaussian integral over p we get

$$\begin{aligned}
\langle x_f, t_f | x_i, t_i \rangle &= \sqrt{\frac{-im}{2\pi\hbar T}} \exp\left(i\frac{mX^2}{2\hbar T} \right) \\
&= \sqrt{\frac{-im}{2\pi\hbar T}} \exp\left(i\frac{S_{cl}}{\hbar} \right)
\end{aligned} \tag{3.14}$$

Comparing (3.14) with (3.11), we see that

$$\det J \prod_{n=1}^{\infty} \int dc_n \exp\left\{ i(m\pi^2/2\hbar T) n^2 c_n^2 \right\} \;=\; \sqrt{\frac{-im}{2\pi\hbar T}}. \tag{3.15}$$

We will use this result in the next example.

[4]This looks like a "circular argument" but we will only use this in the case of a free particle. The jacobian will then be determined for consideration in any other system.

3.2 Example 2: The Harmonic Oscillator

For a particle of mass m performing oscillations in one dimension with angular frequency ω, the Lagrangian is given by

$$L = \frac{m}{2}\dot{x}^2 - \frac{\omega^2}{2}x^2 \tag{3.16}$$

The classical path is

$$x(t) = A\sin(\omega t + \phi) \tag{3.17}$$

where the two constants A and ϕ are chosen such that

$$\begin{aligned} A\sin(\omega t_i + \phi) &= x_i \\ A\sin(\omega t_f + \phi) &= x_f, \end{aligned}$$

so that the particles passes though x_i at time t_i and x_f at time t_f. The classical action is given by

$$S_{cl} = \frac{A^2\omega}{2}\cos(\phi)\sin(\omega T), \tag{3.18}$$

where for convenience we have moved the time origin such that $t_i = -T/2$, $t_f = +T/2$.

The general path may again be given by

$$x(t) = x_{cl}(t) + \sum_{n=1}^{\infty} c_n \phi_n(t) \tag{3.19}$$

where $\phi_n(t)$ are the eigenfunctions of the operator

$$\hat{\mathcal{O}} = -\frac{m}{2}\left(\frac{d^2}{dt^2} + \omega^2\right)$$

The eigenfunctions (which vanish for $t = t_i$ and $t = t_f$) are again given by Eq.(3.9), but the eigenvalues are given by

$$\lambda_n = \frac{m}{2}\left(\frac{n^2\pi^2}{T^2} - \omega^2\right),$$

so that the expression (3.12) for the transition amplitude $\langle x_f, t_f | x)_i, t)_i\rangle$ for a free particle becomes

$$\langle x_f, t_f | x_i, t_i\rangle = \exp\left(i\frac{S_{cl}}{\hbar}\right)\det J \prod_{n=1}^{\infty}\sqrt{\frac{-i\hbar T}{2\pi m}}\,2\left(n^2 - \frac{\omega^2 T^2}{\pi^2}\right)^{-1/2}, \tag{3.20}$$

with S_{cl} given by (3.18). If we rewrite this as

$$\langle x_f, t_f | x_i, t_i\rangle = \exp\left(i\frac{S_{cl}}{\hbar}\right)\det J \prod_{n=1}^{\infty}\sqrt{\frac{-i\hbar T}{2\pi m}}\,\frac{2}{n}\prod_{l=1}^{\infty}\left(1 - \frac{\omega^2 T^2}{\pi^2 l^2}\right)^{-1/2} \tag{3.21}$$

Using (3.15) and the product

$$\prod_{n=1}^{\infty}\left(1-\frac{y^2}{n^2}\right) \;=\; \frac{\sin(\pi y)}{\pi y},$$

We obtain for the harmonic oscillator

$$\langle x_f, t_f \big| x_i, t_i > = \sqrt{\frac{-im\omega}{2\pi\hbar}}\exp\left(i\frac{S_{cl}}{\hbar}\right)\left(\sin(\omega T)\right)^{-1/2} \tag{3.22}$$

We note that if we expand this in powers of $e^{i\omega T}$ we find

$$\langle x_f, t_f \big| x_i, t_i > = \sqrt{\frac{-im\omega}{2\pi\hbar}}\exp\left(i\frac{S_{cl}}{\hbar}\right)\sum_{r=0}^{\infty}\frac{(2r-1)!}{r!(r-1)!2^{(2r-1)}}e^{-i(2r+1/2)\omega T}, \tag{3.23}$$

i.e. we get get terms whose t dependence are $e^{-iE_{2r}T/\hbar}$, where E_{2r} are the (even) energy levels of the harmonic oscillator.[5]

3.3 Imaginary Time

We can dispense with the cumbersome factors of i and their square roots by moving to imaginary time $\tilde{\tau} = -it$. The coordinates $\mathbf{q}$ are now functions of a parameter τ, which does not have a direct physical interpretation. The Lagrangian, $L\left(\mathbf{q}, \dot{\mathbf{q}}\right)$ is replaced by the effective Hamiltonian

$$H_{\text{eff}}(\mathbf{q}, d\mathbf{q}/d\tilde{\tau}) \;\equiv -L\left(\mathbf{q}, i\frac{d\mathbf{q}}{dt}\right)$$

whose action is

$$S_E[q(\tilde{\tau})] \equiv \int_{\mathbf{q}_i}^{\mathbf{q}_f} H_{\text{eff}}\left(\mathbf{q}, d\mathbf{q}/d\tilde{\tau}\right)) \, d\tilde{\tau}$$

In thermal physics the variable $\tilde{\tau}$ is replaced by the inverse of the temperature (in units of the Boltzmann constant). The classical dependence of $\mathbf{q}$ on τ, $\mathbf{q}_{cl}(\tilde{\tau})$, is the function which minimises this action.

The leading dependence of the evolution amplitude $\langle \mathbf{q}_f, \tau_f \big| \mathbf{q}_i, \tau_i \rangle$ is now

$$\exp\left(-\frac{S_E[\mathbf{q}_{cl}(\tilde{\tau})]}{\hbar}\right)$$

For the case of the harmonic oscillator Eq.(3.22) becomes

$$\langle x_f, \tau_f \big| x_i, \tau_i > = \sqrt{\frac{m\omega}{2\pi\hbar}}\exp\left(-\frac{S_E[x_{cl}]}{\hbar}\right)\left(\sinh(\omega\tau)\right)^{-1/2}, \tag{3.24}$$

[5]The odd energy levels are absent because the corresponding eigenfunctions do not satisfy the required boundary conditions.

with $\tau \equiv \tau_f - \tau_i$ and S_{cl}^E means the Euclidean action with the classical path, $\mathbf{q}_{cl}(\tilde{\tau})$.

One immediate consequence of this Euclidean formalism is that the τ-dependence is a series of terms with τ-dependence

$$e^{-E_r\tau/\hbar}$$

where E_r are the energy levels of the system. As $\tau \to \infty$, this is dominated by the ground state energy, and so for large τ we obtain the evolution amplitudes for the ground-state of the system.

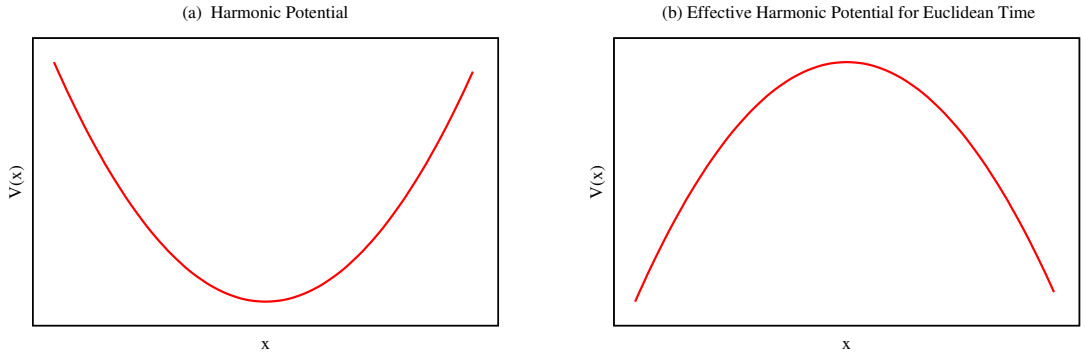

Figure 2: Fig.(a) shows the normal harmonic potential, whereas Fig.(b) shows the effective potential in imaginary time.

In the case of the harmonic oscillator, the classical path $x_{cl}(t) = A\sin(\omega t + \phi)$, describes a particle performing harmonic motion about the minimum of a potential well

$$V(x) \;=\; \frac{1}{2}m\omega^2 x^2.$$

In imaginary time the classical path is $x_{cl}(\tilde{\tau}) = A\sinh(\omega\tilde{\tau} + \phi)$, describing a particle moving in a potential hump

$$V(x) \;=\; -\frac{1}{2}m\omega^2 x^2.$$

and the action is

$$S_E \;=\; \frac{A}{2}\omega^2\cosh(\phi)\sinh(\omega\tau)$$

As the imaginary time-interval $\tau \to \infty$ the action is minimised by setting the "amplitude" A to zero. For any other path the distance $\left|x_f - x_i\right|$ must grow exponentially as $\tau \to \infty$ representing a particle rolling down a the potential hump. For $A = 0$, the action is zero and so in this limit we may omit the factor $\exp\left(-S_E/\hbar\right)$.

4 Correlators

A quantity which is often very useful is the correlator, which is the expectation value of a product of the coordinates at given times. e.g.

$$\langle \mathbf{q}_i, t_i \big| T\hat{\mathbf{q}}(t_2)\hat{\mathbf{q}}(t_1)\cdots\hat{\mathbf{q}}(t_k)\big|\mathbf{q}_i, t_i\rangle.$$

Here the symbol T means time-ordered and it means that $t_1 > t_2 > \cdots > t_k$. Note also that we have written $\mathbf{q}$ as an operator at a given time (Heisenberg representation).

Inserting complete sets of states at times $t_1, t_2, \cdots t_k$, we get

$$\begin{aligned}\langle \mathbf{q}_i, t_i \big| T\hat{\mathbf{q}}(t_2)\hat{\mathbf{q}}(t_1)\cdots\hat{\mathbf{q}}(t_k)\big|\mathbf{q}_i, t_i\rangle \;\; &= \\ \int d^d\mathbf{q}_1 d^d\mathbf{q}_2 \cdots d^d\mathbf{q}_k \, \mathbf{q}_1\mathbf{q}_2\cdots\mathbf{q}_k \langle \mathbf{q}_f, t_f\big|\mathbf{q}_1, t_1\rangle\langle \mathbf{q}_1, t_1\big|\mathbf{q}_2, t_2\rangle\cdots\langle \mathbf{q}_k, t_k\big|\mathbf{q}_i, t_i\rangle &(4.1)\end{aligned}$$

since $\langle \mathbf{q}_1, t_1\big|\mathbf{q}_2, t_2\rangle$ means sum over all paths between t_2 and t_1 whose values are fixed at those times, we can write the product on the transition amplitudes as an integral over *all* paths with appropriate δ-functions at $t_1, t_2, \cdots t_k$ so that we have

$$\begin{aligned}\langle \mathbf{q}_i, t_i \big| T\hat{\mathbf{q}}(t_2)\hat{\mathbf{q}}(t_1)\cdots\hat{\mathbf{q}}(t_k)\big|\mathbf{q}_i, t_i\rangle \;\; &= \\ \int d^d\mathbf{q}_1 d^d\mathbf{q}_2 \cdots d^d\mathbf{q}_k \int_{\mathbf{q}_i,t_i}^{\mathbf{q}_f,t_f} \mathcal{D}[\mathbf{q}(t)]\mathbf{q}_1\mathbf{q}_2\cdots\mathbf{q}_k \exp\left\{\frac{i}{\hbar}S[\mathbf{q}(t)]\right\} & \\ \delta^d\left(\mathbf{q}(t_1)-\mathbf{q}_1\right)\delta^d\left(\mathbf{q}(t_2)-\mathbf{q}_2\right)\cdots\delta^d\left(\mathbf{q}(t_k)-\mathbf{q}_k\right) &(4.2)\end{aligned}$$

We use the integrations over $\mathbf{q}_i$ etc. to absorb the δ-functions, so that finally we have

$$\begin{aligned}\langle \mathbf{q}_i, t_i \big| T\hat{\mathbf{q}}(t_2)\hat{\mathbf{q}}(t_1)\cdots\hat{\mathbf{q}}(t_k)\big|\mathbf{q}_i, t_i\rangle \;\; &= \\ \int \mathcal{D}[\mathbf{q}(t)]\mathbf{q}(t_1)\mathbf{q}(\mathbf{t_2})\cdots\mathbf{q}(\mathbf{t_k})\exp\left\{\frac{i}{\hbar}S[\mathbf{q}(t)]/\hbar\right\} &(4.3)\end{aligned}$$

There is a convenient trick for determining these path integrals, by introducing a source function $\mathbf{j}(t)$ and adding the term

$$\int_{t_i}^{t_f}\mathbf{j}(t)\cdot\mathbf{q}(t)dt$$

to the effective action so that we obtain the source-dependent evolution amplitude

$$\langle \mathbf{q}_f, t_f\big|\mathbf{q}_i, t_i\rangle_{\mathbf{j}} \;=\; \int_{t_i}^{t_f}\mathcal{D}[\mathbf{q}(t)]\exp\left\{\frac{i}{\hbar}\left(S[\mathbf{q}(t)+\int_{t_i}^{t_f}\mathbf{j}(t)\cdot\mathbf{q}(t)\right)\right\}, \qquad (4.4)$$

so that factors of $\mathbf{q}(t_1)$ etc. can be wrought into the path integral by performing a functional integral w.r.t. to the source function, and then setting the source function to zero, i.e.

$$\begin{aligned}\int \mathcal{D}[\mathbf{q}(t)]\mathbf{q}(t_1)\mathbf{q}(\mathbf{t_2})\cdots\mathbf{q}(\mathbf{t_k})\exp\left(i\frac{S[\mathbf{q}(t)]}{\hbar}\right) \;\; &= \\ \left(-i\hbar\frac{\delta}{\delta\mathbf{j}(t_1)}\right)\left(-i\hbar\frac{\delta}{\delta\mathbf{j}(t_2)}\right)\cdots\left(-i\hbar\frac{\delta}{\delta\mathbf{j}(t_k)}\right)\langle \mathbf{q}_f, t_f\big|\mathbf{q}_i, t_i\rangle_{\mathbf{j}=0} &(4.5)\end{aligned}$$

Restricting ourselves to one dimension, We can once again write the general path as

$$x(t) \;=\; x_{cl}(t) + \sum_n c_n \phi_n(t),$$

so that in the presence of a source the path integral is

$$\langle x_f, t_f | x_i, t_i \rangle_j \;=\; \exp\left\{\frac{i}{\hbar}\left(S_{cl} + \int_{t_i}^{t_f} j(t) x_{cl}(t)\right)\right\} detJ \prod_{n=1}^{\infty} \int dc_n \exp\left\{\frac{i}{\hbar}(\lambda_n c_n^2 + c_n \int_{t_i}^{t_f} dt j(t)\phi_n(t)\right\}, . \tag{4.6}$$

where λ_n are the eigenvalues of the operator $\hat{\mathcal{O}}$ The Gaussian integral over the coefficient c_n can again be performed yielding

$$\begin{aligned}\langle x_f, t_f | x_i, t_i \rangle_j \;&=\; \exp\left\{\frac{i}{\hbar}\left(S_{cl} + \int_{t_i}^{t_f} j(t) x_{cl}(t)\right)\right\} detJ \\ &\prod_{n=1}^{\infty} \sqrt{\frac{-i2\pi}{\lambda_n}} \exp\left\{-\frac{i}{\hbar}\int_{t_i}^{t_f} dt dt' \frac{j(t)\phi_n(t) j(t')\phi_n(t')}{\lambda_n}\right\}\end{aligned} \tag{4.7}$$

We can write

$$\prod_{n=1}^{\infty} \exp\left\{-\frac{i}{\hbar}\int_{t_i}^{t_f} dt dt' \frac{j(t)\phi_n(t) j(t')\phi_n(t')}{\lambda_n}\right\} \;=\; \exp\left\{-\frac{i}{\hbar}\int_{t_i}^{t_f} dt dt' j(t)\hat{\mathcal{O}}^{-1}_{(t,t')} j(t')\right\}, \tag{4.8}$$

where $\hat{\mathcal{O}}^{-1}$ is the inverse of the operator $\hat{\mathcal{O}}$, which obeys the Green-function equation

$$\hat{\mathcal{O}}(t)\hat{\mathcal{O}}^{-1}(t,t') \;=\; \delta(t-t'). \tag{4.9}$$

This inverse operator may be written

$$\hat{\mathcal{O}}^{-1}(t,t') \;=\; \sum_{n=1}^{\infty} \frac{\phi_n^*(t)\phi_n(t')}{\lambda_n}. \tag{4.10}$$

Operating on both sides of (4.10) and using the completeness relation for the eigenfunctions ϕ_n we get

$$\hat{\mathcal{O}}(t)\hat{\mathcal{O}}^{-1}(t,t') \;=\; \sum_{n=1}^{\infty} \phi_n^*(t)\phi_n(t') \;=\; \delta(t-t'). \tag{4.11}$$

Note that each application of a functional derivative w.r.t. the source $j(t)$ brings down an expected factor of $x_{cl}(t)$, as expected, plus a quantum correction which is proportional to $\sqrt{\hbar}$, and therefore vanishes in the classical limit.

5 Semi-classical approximation

So far, we have succeeded in determining the evolution functions by performing the necessary path integrals exactly. We have been able to do this because the Lagrangian in the examples

considered are quadratic in the coordinate or velocity. In such cases the action for a general path is given exactly by

$$S[x(t)] = S_{cl} + \frac{1}{2}\int_{t_i}^{t_f} dt dt' \frac{\delta^2 S_{cl}}{\delta x_{cl}(t)\delta x_{cl}(t')} x_{qu}(t) x_{qu}(t') \tag{5.1}$$

The operator $\hat{\mathcal{O}}$ is given by

$$\hat{\mathcal{O}}(t)\delta(t-t') \;=\; \frac{\delta^2 S_{cl}}{\delta x_{cl}(t)\delta x_{cl}(t')}.$$

Note that there is *no* term linear in x_{qu} because x_{cl} is the path which minimises the action.

However, for a general system for which the Lagrangian contains higher powers of the coordinates and/or velocities, we expect the action for a given path to be of the form (again restricting ourselves to one dimension)

$$S[x(t)] \;=\; S_{cl} + \int_{t_i}^{t_f} dt \hat{\mathcal{O}} x_{qu}(t)^2 + \sum_{r=3} \int_{t_i}^{t_f} dt_1 dt_2 \cdots dt_r S_r(t_1, t_2 \cdots t_r) x_{qu}(t) x_{qu}(t_2) \cdots x_{qu}(t_r), \tag{5.2}$$

where

$$S_r(t_1, t_2 \cdots t_r) \;\equiv\; \frac{1}{r!}\frac{\delta^r S_{cl}}{\delta x_{cl}(t_1)\cdots\delta x_{cl}(t_r)}.$$

S_r is in general a function of the times $t_1 \cdots t_r$ and possibly also the derivative operators $d/dt_1 \cdots d/dt_r$.

If these terms are sufficiently small, we may neglect them and just consider the term in the action which is quadratic in x_{qu}. This is called the "semi-classical approximation". In this approximation we expand the classical action only to second order in the quantum correction, x_{qu} and integrate the gaussian integral over x_{qu} to obtain (up to an overall constant)

$$\langle x_f, t_f \big| \hat{x}(t_1) \cdots \hat{x}(t_k) \big| x_i, t_i \rangle \;=\; \left(\det \left\{ \frac{\hat{\mathcal{O}}}{2\pi\hbar} \right\} \right)^{-1/2} x_{cl}(t_1) \cdots x_{cl}(t_k) \exp\left(\frac{i}{\hbar} S_{cl} \right), \tag{5.3}$$

where

$$S_{cl} \;=\; \int_{t_i}^{t_f} L\left(x_{cl}(t), \dot{x}_{cl}(t)\right) \tag{5.4}$$

and $\det \hat{\mathcal{O}}$ is the product of all eigenvalues with eigenfunctions that vanish at $t = t_i$ and $t = t_f$.

There is a clever trick for calculating the determinant of an operator which is second order in the time-derivative, $\hat{\mathcal{O}}$. For any value of λ there exists a function $x_\lambda(t)$ such that

$$\frac{1}{2\pi\hbar}\hat{\mathcal{O}} x_\lambda(t) = \lambda x_\lambda(t),$$

which vanishes as $t = t_i$, but in general it does *not* vanish at $t = t_f$ unless λ is equal to one of the eigenvalues λ_n. To fix the normalisation of x_λ we will also impose the initial condition

$$\frac{d}{dt}x_\lambda(t_i) = 1.$$

Now consider two different operators $\hat{\mathcal{O}}_1$ and $\hat{\mathcal{O}}_2$ and the function of λ

$$\frac{\det(\hat{\mathcal{O}}_1/2\pi\hbar - \lambda\mathbb{1})}{\det(\hat{\mathcal{O}}_2/2\pi\hbar - \lambda\mathbb{1})}$$

This is equal to

$$\frac{x_{\lambda,1}(t_f)}{x_{\lambda,2}(t_f)}.$$

We can see this because both sides have zeroes when $\lambda = \lambda_n$, the eigenvalues of $\hat{\mathcal{O}}$, and poles when $\lambda = \lambda'_n$, the eigenvalues of $\hat{\mathcal{O}}'$. Both sides tend to unity in the limit $\left|\lambda\right| \to \infty$. The functions are therefore identical. Setting λ to zero we therefore find

$$\frac{\det\left(\hat{\mathcal{O}}_1/2\pi\hbar\right)}{x_{0,1}(t_f)} = \frac{\det\left(\hat{\mathcal{O}}_2/2\pi\hbar\right)}{x_{0,2}(t_f)} \;=\; N, \tag{5.5}$$

where N is a constant.

In the case of a free particle we find

$$x_0(t) \;=\; (t - t_i), \tag{5.6}$$

so that

$$\left(\det\left\{\frac{\hat{\mathcal{O}}}{2\pi\hbar}\right\}\right)^{-1/2} \propto T^{-1/2},$$

which is consistent with (3.15), whereas for a harmonic oscillator we find

$$x_0(t) \;=\; \sin\left(\omega(t - t_i)\right), \tag{5.7}$$

so that for the harmonic oscillator

$$\left(\det\left\{\frac{\hat{\mathcal{O}}}{2\pi\hbar}\right\}\right)^{-1/2} \propto \sin(\omega T)^{-1/2},$$

which is consistent with (3.22).

More generally, for a particle of mass m moving in a potential $V(x)$, the operator $\hat{\mathcal{O}}$ takes the form

$$\hat{\mathcal{O}} \;=\; \frac{m}{2}\frac{d^2}{dt^2} + V''(x_{cl}) \tag{5.8}$$

the solution with $\lambda = 0$ is given by

$$x_0(t) \;=\; \dot{x}_{cl}(t_i)\dot{x}_{cl}(t)\int_{x_i}^{x_{cl}(t)} dx \frac{1}{(\dot{x})^3}. \tag{5.9}$$

Using

$$V''(x_{cl}) \;=\; -\frac{m}{\dot{x}_{cl}}\frac{d^3x_{cl}}{dt^3}, \tag{5.10}$$

we can see that

$$\frac{d^2}{dt^2}x_0(t) + V''(x_{cl})x_0(t) \;=\; 0, \tag{5.11}$$

(we also see that (7.9) the required boundary values at $t = t_i$.) Thus we have the result

$$\det\left\{\frac{\hat{\mathcal{O}}}{2\pi\hbar}\right\} \;=\; \dot{x}_{cl}(t_i)\dot{x}_{cl}(t_f)\int_{x_i}^{x_f} dx \frac{1}{(\dot{x})^3} \tag{5.12}$$

(up to an overall constant), and so finally we have for the path integral in the semi-classical approximation

$$\langle x_f, t_f | x_i t_i\rangle \;=\; \sqrt{\frac{2\pi}{N}}\left(\dot{x}_{cl}(t_i)\dot{x}_{cl}(t_f)\int_{x_i}^{x_f} dx \frac{1}{(\dot{x})^3}\right)^{-1/2} \exp\left\{\frac{i}{\hbar}S_{cl}\right\} \tag{5.13}$$

It may be the case that there exists more than one classical path $\mathbf{q}(t)$, with boundary values $\mathbf{q}(t_i) = \mathbf{q}_i$, $\mathbf{q}(t_f) = \mathbf{q}_f$. These paths are not necessarily minima of the action, but merely turning-points, or saddle-points. In this case the path-integral is given in the semi-classical approximation by the sum of the terms obtained by expanding the coordinates to quadratic order about each saddle-point. For this reason the semi-classical approximation is also known as the saddle-point approximation.

In one dimension, we may have a series of classical paths, $x^k_{cl}(t)$, with corresponding actions S^k_{cl} and quadratic operators $\hat{\mathcal{O}}^k$

$$\hat{\mathcal{O}}^k(t)\delta(t-t') \;=\; \frac{\delta^2 S^k_{cl}}{\delta x^k_{cl}(t)\delta x^k_{cl}(t')}.$$

The semi-classical approximation to the transition amplitude is then

$$\langle x_f t_i | x_i, t_i\rangle \;=\; \sum_k \left[\left(\det\left\{\frac{\hat{\mathcal{O}}^k}{2\pi\hbar}\right\}\right)^{-1/2} \exp\left\{\frac{i}{\hbar}S^k_{cl}\right\}\right] \tag{5.14}$$

5.1 Equivalence with WKB approximation

We consider a particle of mass m moving in one dimension in a potential $V(x)$ with energy E. In the WKB approximation gives the (time-dependent) wavefunction

$$\Psi_E(x,t) = \frac{1}{\sqrt{p_E(x)}} \exp\left\{\frac{i}{\hbar}\left(\int_{x_0}^{x} p_E(x')dx' - Et\right)\right\}, \tag{5.15}$$

where the "momentum" $p_E(x)$ is given by

$$p_E(x) = \pm\sqrt{2m(E - V(x))} \tag{5.16}$$

and the lower limit of the integral, x_0 is selected to give rise to a properly normalised wavefunction. Note that in regions of x where $V(x) > E$ this momentum is purely imaginary and we get a wavefunction which decreases exponentially with x. Although a classical particle cannot propagate in a such a region, in quantum physics this can happen and the wavefunction describes quantum tunnelling.

The evolution amplitude from (x_i, t_i) to (x_f, t_f) can be written in terms of a complete set of energy eigenvalues

$$\langle x`_f, t_f \big| x_i, t_i \rangle \;=\; \int dE \Psi^*_E(x_f, t_f)\Psi_E(x_i, t_i) \tag{5.17}$$

In the WKB approximation (5.15) this becomes

$$\langle x`_f, t_f \big| x_i, t_i \rangle \;=\; \int dE \frac{1}{\sqrt{p_E(x_f)p_E(x_i)}} \exp\left\{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p_E(x')dx' - E(t_f - t_i)\right)\right\}, \tag{5.18}$$

with $p_E(x)$ being a function of x and E given by (5.16). Note that in the integral over E only one value corresponds to the classical value, E_{cl}, which is the energy such the classical path passes through the two points x_i, t_i and x_f, t_f, namely the energy for which

$$t_f - t_i \;= m\int_{x_i}^{x_f} dx' \frac{1}{p_{E_{cl}}(x')} \tag{5.19}$$

Once again, we can perform the integral over E using the "saddle-point" approximation, namely we write

$$E = E_{cl} + \delta E \tag{5.20}$$

and expand the exponent, $S(E)$, in (5.18) up to quadratic order in δE, In the pre-factor we set p_E to $p_{E_{cl}}$. Expanding the exponent to quadratic order

$$S(E) = \frac{i}{\hbar}\left(\int_{x_i}^{x_f} dx' p_{E_{cl}}(x') - E_{cl}(t_f - t_i)\right) + \mathcal{M}(\delta E)^2, \tag{5.21}$$

with

$$\mathcal{M} \;= \frac{i}{2\hbar}\frac{d^2}{dE^2}\left\{\int_{x_i}^{x_f} \sqrt{2m(E - V(x'))}dx' - E(t_f - t_i)\right\} \;=\; -\frac{im^2}{2\hbar}\int_{x_i}^{x_f} dx' \frac{1}{p_{E_{cl}}(x')^3} \tag{5.22}$$

We can perform the gaussian integral over δE which introduces a factor

$$\left(\frac{i}{4\pi i}\frac{m^2}{\hbar}\int_{x_i}^{x_f} \frac{dx'}{p_{E_{cl}}(x')^3}\right)^{-1/2}$$

Piecing this together and inserting into (5.18) we get

$$\langle x_f, t_f \big| x_i, t_i \rangle \;=\; c \left(p_{E_{cl}}(x_f) p_{E_{cl}}(x_i) \int_{x_i}^{x_f} dx' \frac{1}{p_{E_{cl}}(x')^3} \right)^{-1/2} \exp\left\{ \frac{i}{\hbar} \left(\int_{x_i}^{x_f} p_{E_{cl}}(x') dx' - E_{cl}(t_f - t_i) \right) \right\}, \tag{5.23}$$

where the overall constant c is determined by the requirement

$$\lim_{t_f \to t_i} \langle x_f, t_f \big| x_i, t_i \rangle \;=\; \delta(x_i - x_f).$$

We can write

$$\int_{x_i}^{x_f} dx' p_{E_{cl}}(x') = \int_{t_i}^{t_f} p_{E_{cl}}(x_{cl}(t)) \dot{x}_{cl}(t)\, dt$$

and replace the classical energy E_{cl} by the Hamiltonian, H, as a function of $p_{E_{cl}}$ and x_{cl}, so that the exponent in (5.23) becomes

$$\frac{i}{\hbar} \int_{t_0}^{t} (p_E(x_{cl}(t)) \dot{x}_{cl}(t) - H(p_{E_{cl}}(x(t), x(t)\, dt) \;\equiv\; \frac{i}{\hbar} \int_{t_0}^{t} L(x_{cl}(t), \dot{x}_{cl}(t))\, dt \;=\; \frac{i}{\hbar} S_{cl},$$

so that finally we get (using $p_{E_{cl}}(x_{cl}(t)) = m\dot{x}_{cl}$)

$$\langle x_f, t_f \big| x_i, t_i \rangle \;=\; \frac{c}{m} \left(\dot{x}_{cl}(t_f) \dot{x}_{cl}(t_i) \int_{x_i}^{x_f} dx \frac{1}{\dot{x}^3} \right)^{-1/2} \exp\left\{ \frac{i}{\hbar} S_{cl} \right\}, \tag{5.24}$$

which is identical to the expression (5.13) obtained from the approximation to the path integral in the semi-classical approximation.

6 Perturbation Theory

If we wish to calculate the evolution amplitudes beyond the semi-classical approximate, then, provided the coefficients of these higher order terms are sufficiently small, we can expand the exponential of these higher terms as a power series in the coefficients S_r such that

$$\begin{aligned} \exp\left(i \frac{S[x(t)]}{\hbar} \right) \;&=\; \exp\left(i \frac{S_{cl}}{\hbar} \right) \exp\left\{ \frac{i}{\hbar} \int_{t_i}^{t_f} dt \hat{\mathcal{O}} x_{qu}(t)^2 \right\} \\ &\times \left[1 + \sum_{r=3} \frac{i}{\hbar} \int_{t_i}^{t_f} dt_1 dt_2 \cdots dt_r S_r(t_1, t_2 \cdots t_r) x_{qu}(t) x_{qu}(t_2) \cdots x_{qu}(t_r) + \cdots \right] \end{aligned} \tag{6.1}$$

Up to any given order in the coefficients the transition amplitude can be calculated by calculating the required correlators, in which appropriate multiples of the coordinate at various given times multiplies the integrand in the path integral (see (4.3)). Note that despite the factor of $1/\hbar$ for each power of the coefficients S_r, we have a factor of $\sqrt{\hbar}$ for each factor of the coordinate in the correlator function, and so this perturbative expansion is

an expansion in powers of $\hbar$ and the sub-leading terms constitute quantum corrections. For example if the Lagrangian contains a quartic term S_4, the contribution to the path integral from such a term is suppressed by a factor of

$$\frac{1}{\hbar}\left(\sqrt{\hbar}\right)^4 = \hbar$$

and higher order terms are even further suppressed.

7 Instantons in Quantum Mechanics

7.1 Double well potential

Consider a particle of mass m moving in a one-dimensional double-well potential

$$V(x) = \frac{m\omega^2}{8\lambda^2}\left(x^2-\lambda^2\right)^2 \tag{7.1}$$

This is a double well potential shown in the left diagram of Fig.3

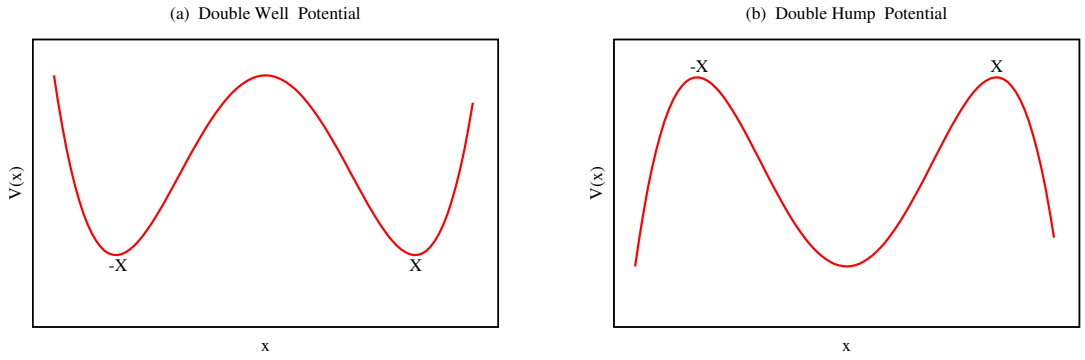

Figure 3: Fig.(a) shows a double well potential. Fig(b) shows the corresponding effective double hump potential in Eucidean time.

Near the points $x = \lambda$ and $x = -\lambda$, the potential behaves like a harmonic oscillator

$$V(x) \approx \frac{m\omega^2}{2}(\Delta x)^2$$

with $\Delta x = (x \pm \lambda)$.

At first sight, it may seem that the spectrum of states is just two degenerate sets of harmonic oscillator energy levels - at least for the lower energy levels where the particle is most likely to be found close to the potential minimum at $x = \lambda$ or $x = -\lambda$. However, in Quantum Physics a particle which starts off at $x = -x$ can tunnel through the barrier to the point $x = +\lambda$ or *vice versa*.

The quantum amplitude for such a transition is

$$\langle \lambda, \frac{T}{2} | -\lambda, -\frac{T}{2} \rangle \;=\; \int \mathcal{D}[x(t)] \exp\left\{ \frac{i}{\hbar} S^{\lambda}_{-\lambda}[x(t)]] \right\}, \tag{7.2}$$

where $S^{\lambda}_{\lambda}[x(t)]$ is the action due to the path $x(t)$ which has the value $x = -\lambda$ at $t = -T/2$ and $x = \lambda$ at time $T/2$.

The best way to perform the path integrals to move to imaginary time $t \to i\tilde{\tau}$ so that the effective potential is the double-hump potential shown on the right of Fig.3. Although there is no classical path in real time that can be taken by a particle to get from $-\lambda$ to λ, in imaginary time the equation of motion

$$\frac{d^2}{d\tilde{\tau}^2} x(\tilde{\tau}) \;=\; \frac{\omega^2}{2\lambda^2}(x^2 - \lambda^2)x \tag{7.3}$$

has a solution

$$x_I(\tilde{\tau}) \;=\; \lambda \tanh\left(\frac{\omega\tilde{\tau}}{2}\right), \tag{7.4}$$

which has boundary values

$$\lim_{\tilde{\tau}\to\pm\infty} \;=\; \pm\lambda,$$

so it describes a particle moving in the double hump potential between $x = -\lambda$ as $\tau \to -\infty$ and $x = +\lambda$ as $\tau \to +\infty$, as shown in Fig.4.

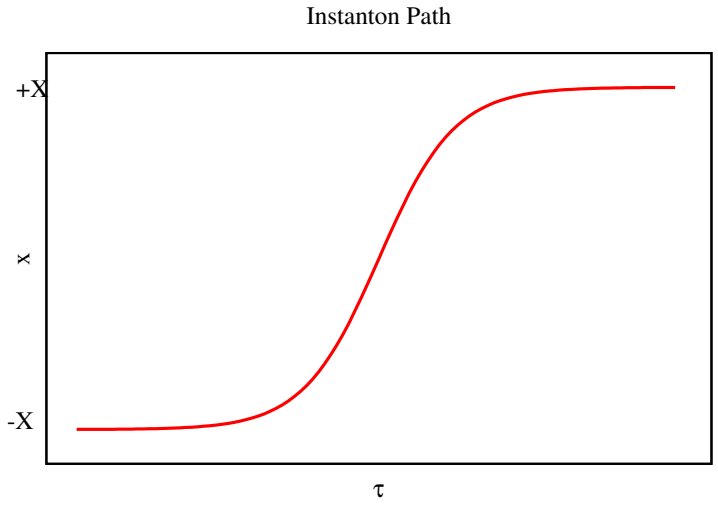

Figure 4: Instanton path. $x(\tau) \to -\lambda$ as $\tau \to -\infty$ and $x(\tau) \to +\lambda$ as $\tau \to +\infty$

This class of x_{cl}, whose limits $\tilde{\tau} \to \pm\infty$ correspond to different minima of the potential, is called an "instanton" (hence the notation x_I for this classical path).

As it is a solution of the equation of motion, it gives rise to the minimum action, (the classical action) S_I, in imaginary time, given by

$$S_I \;=\; \int_{-\tau/2}^{\tau/2} (x_I(\tilde{\tau}))^2 \, d\tilde{\tau} \;=\; \int_{-\tau/2}^{\tau/2} \frac{m\omega^2\lambda^2}{4\cosh^4(\omega\tilde{\tau}/2)} d\tilde{\tau} \;\approx\; \frac{2}{3} m\omega\lambda^2 \text{ (for } \omega\tau \gg 1). \tag{7.5}$$

We can then calculate the path integral approximately in the semi-classical approximation.

The transition amplitude contains a factor (the barrier penetration factor)

$$e^{-S_I/\hbar} \;=\; \exp\left\{-\frac{2m\omega\lambda^2}{3\hbar}\right\}$$

Note that in a macroscopic system $S_I \gg \hbar$, so that the tunnelling amplitude is negligibly small.

7.2 Zero Modes

In order to compute the path integral in (7.2) we need the determinant of the operator

$$\hat{\mathcal{O}} \;=\; \frac{d^2}{d\tilde{\tau}^2} + V''(x_I(\tilde{\tau}) \;= \frac{d^2}{d\tilde{\tau}^2} + \frac{m\omega^2}{2}\left(3\tanh^2\left(\frac{\omega\tilde{\tau}}{2}\right) - 1\right) \tag{7.6}$$

But this operator has a zero mode (an eigenfunction with eigenvalue zero)

$$x_0(\tilde{\tau}) \;=\; \sqrt{\frac{3\omega}{8}} \frac{1}{\cosh^2(\omega\tilde{\tau}/2)} \tag{7.7}$$

This arises because a more general instanton solution, specifies the imaginary time τ_c, at which $x_I = 0$ (the "centre" of the instanton where $x_I(\tau) = 0$) takes the value τ_c.

$$x_{I_{\tau_c}}(\tilde{\tau}) \;=\; \lambda \tanh\left(\frac{m\omega(\tilde{\tau} - \tau_c)}{2}\right) \tag{7.8}$$

The Lagrangian is originally invariant under time transformation

$$L\left(x(\tilde{\tau}), \dot{x}(\tilde{\tau})\right) \;=\; L\left(x(\tilde{\tau} + \Delta\tau), \dot{x}(\tilde{\tau} + \Delta\tau)\right).$$

By specifying the instanton centre, τ_c this symmetry is spontaneously broken and (in analogy with Goldstone bosons) there is a mode with arbitrarily small energy, corresponding to the infinitesimally slow movement of the instanton centre. This zero mode is given by the rate of change of the instanton configuration, $x_{I_{\tau_c}}$, with respect to τ_c. From (7.4),(7.5) and (7.7) the normalised zero mode is

$$x_0(\tilde{\tau}) \;=\; \sqrt{\frac{m}{S_I}} \frac{d}{d\tau_c} x_{I_{\tau_c}}(\tilde{\tau}) \tag{7.9}$$

The existence of this zero mode means that the determinant of $\hat{\mathcal{O}}$ is zero and the pre-factor $\left(\det\left\{\hat{\mathcal{O}}/2\pi\hbar\right\}\right)^{-1/2}$ diverges.

For the moment we will not eliminate this problem, but we will factor out the coefficient, c_0, of the zero mode in the expansion of $x(\tilde{\tau})$ as a sum of eigenfunctions of $\hat{\mathcal{O}}$. The pre-factor is then

$$\left(\det\left\{\frac{\hat{\mathcal{O}}'}{2\pi\hbar}\right\}\right)^{-1/2} dc_0,$$

where $\det\hat{\mathcal{O}}'$ means the product of all *non-zero* eigenvalues of $\hat{\mathcal{O}}$.

The integral over the coefficient c_0 can be traded for an integral over τ_c (known as a "collective coordinate"). We compare the change in the path from an infinitesimal change, dc_0 in c_0 with that obtained from an infinitesimal change in τ_c . From (7.9) this is

$$dc_0 = \sqrt{\frac{S_I}{m}} d\tau_c \tag{7.10}$$

Let us write the determinant of the reduced operator (with the zero mode removed) as

$$\frac{2\pi\hbar}{S_I}\frac{1}{K^2 m\omega^2}\det\left\{\frac{1}{2\pi\hbar}\left(\frac{d^2}{d\tilde{\tau}^2}-\omega^2\right)\right\}$$

From the treatment of the harmonic oscillator (in imaginary time) we see that (see (3.24))

$$\det\left\{\frac{1}{2\pi\hbar}\left(\frac{d^2}{d\tilde{\tau}^2}-\omega^2\right)\right\} \;=\; \frac{2\pi\hbar}{m\omega}\sinh(\omega\tau). \tag{7.11}$$

The constant, K is given by

$$K \;=\; \eta\sqrt{\frac{S_I}{2\pi\hbar}} \tag{7.12}$$

where the numerical constant η depends on the second derivative of the potential. In the case of the potential (7.1), after many manipulations this number η can be shown to be equal to $\sqrt{12}$.

So that finally we have the amplitude for transition from $(-\lambda, -\tau/2)$ to $(+x, +\tau/2)$ due to a one-instanton path is given in terms of an integral over the collective coordinate τ_c

$$\langle\lambda, \frac{\tau}{2}|-\lambda, -\frac{\tau}{2}\rangle_{1I} \;= \frac{1}{2\pi}\sqrt{\frac{12m\omega}{\hbar}}\sqrt{\frac{S_I}{\hbar}}e^{-S_I/\hbar}\left(\sinh(\omega\tau)\right)^{-1/2}\int\omega d\tau_c \tag{7.13}$$

For sufficiently large τ this may be approximated by

$$\langle\lambda, \frac{\tau}{2}|-\lambda, -\frac{\tau}{2}\rangle_{1I} \;=\; Ke^{-S_I/\hbar}e^{-\omega\tau/2}\int\omega d\tau_c, \tag{7.14}$$

with K given by (7.12).

7.3 Instanton gas

Finally, we address the problem of the apparent divergent generated by integrating over all possible values of the centre of the instanton, τ_c.

We start by noting that we can rewrite Eq.(7.14) as

$$\langle \lambda, \frac{\tau}{2} \big| -\lambda, -\frac{\tau}{2} \rangle_{1I} \;=\; \int \omega d\tau_c \, \rho \, \langle \lambda, \frac{\tau}{2} \big| \lambda, -\frac{\tau}{2} \rangle_{0I} \tag{7.15}$$

where $\langle \lambda, \frac{\tau}{2} \big| \lambda, -\frac{\tau}{2} \rangle_{0I}$ is the amplitude for a transition from $(\lambda, -\tau/2)$ to $\lambda, \tau/2)$ in the absence of an instanton, i.e the amplitude due to just a harmonic oscillator potential for oscillations about $x = \lambda$, and the "instanton density", ρ is given by

$$\rho \;\equiv\; K e^{-S_I/\hbar} \;=\; \sqrt{\frac{6S_I}{\pi\hbar}} e^{-S_I/\hbar}. \tag{7.16}$$

For large τ the zero instanton amplitude is

$$\langle \lambda, \frac{\tau}{2} \big| \lambda, -\frac{\tau}{2} \rangle_{0I} \;=\; \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\omega\tau/2} \tag{7.17}$$

As well as a path consisting of a single instanton with a centre τ_1 we have have a path with an instanton followed (in imaginary time) by an anti-instanton which effects tunnelling back from $+\lambda$ to $-\lambda$. Such a path is given by

$$x_{2I}(\tilde{\tau}) \;=\; \lambda \tanh\left(\frac{1}{2}\omega(\tau_2 - \tilde{\tau})\right) \tanh\left(\frac{1}{2}\omega(\tilde{\tau} - \tau_1)\right) \tag{7.18}$$

This path is shown in Fig.5. It is *not* an exact solution, but a very good approximation to a solution provided the centres of the instanton and anti-instanton are sufficiently widely separated, i.e.

$$\omega \big| \tau_1 - \tau_2 \big| \;\gg\; 1.$$

The amplitude for such a path - an instanton followed by an anti-instanton is given by

$$\langle \lambda, \frac{\tau}{2} \big| \lambda, -\frac{\tau}{2} \rangle_{2I} \;=\; \int_{-\tau/2}^{\tau/2} \omega d\tau_2 \int_{-\tau/2}^{\tau_2} \omega d\tau_1 \, K^2 e^{-2S_I/\hbar} \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left(-\frac{1}{2}\omega\tau\right) \tag{7.19}$$

The integration over the centres of the instantons, τ_1 and τ_2 are ordered because the anti-instanton follows the instanton, so that $\tau_2 > \tau_1$. Near the upper limit of the integral τ_1 i.e. $(\tau_1 \sim \tau_2)$ the approximation used in (7.18) is no-longer valid. However, provided the instanton density ρ is sufficiently small, the region in τ_1, τ_2 space over which (7.18) is invalid is a very small part of the entire area, τ^2. More precisely, (7.18) becomes invalid when $\omega(\tau_2 - \tau_1) \sim 1$ and this is a relatively small region provided $\omega\tau \gg 1$. This approximation is called the "dilute gas approximation".

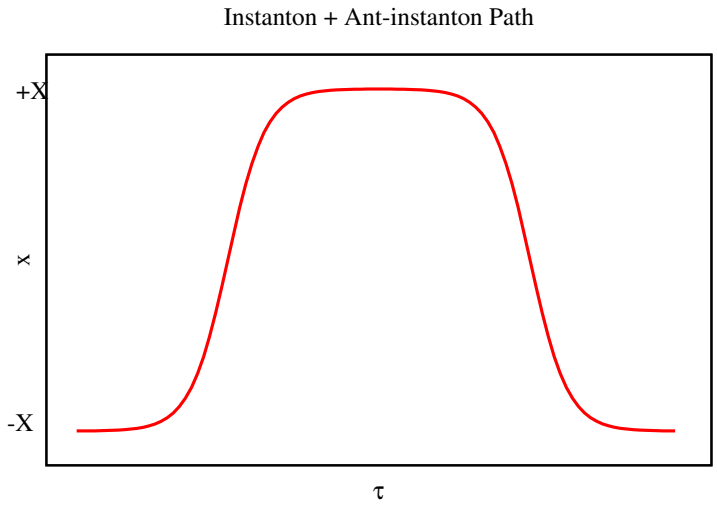

Figure 5: Instanton followed by anti-instanton path.

We can generalise this to n instantons or anti-instantons to get

$$\begin{aligned}\langle\lambda,\frac{\tau}{2}\big|(-1)^n\lambda,-\frac{\tau}{2}\rangle_{nI} \quad &= \\ \int_{-\tau/2}^{\tau/2}\omega d\tau_n\int_{\tau/2}^{\tau_n}\omega d\tau_{n-1}\cdots\int_{-\tau/2}^{\tau_2}\omega d\tau_1\ \left(Ke^{-S_I/\hbar}\right)^n\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2} \qquad &(7.20)\end{aligned}$$

The nested integral over $\tau_1\cdots\tau_n$ gives a factor of

$$\frac{1}{n!}(\omega\tau)^n$$

If n is odd the path effects a transition from $-\lambda$ to λ, and if n is even the path effects a transition from $-\lambda$ to $-\lambda$ or λ to λ. Examples are shown in Fig.6.

As indicated in (5.14), the transition amplitude is obtained in the semi-classical approximation by summing over all the classical paths which pass through the initial and final points.

Summing over all odd n we have

$$\begin{aligned}\langle\pm\lambda,\frac{\tau}{2}\big|\mp\lambda,\frac{-\tau}{2}\rangle \quad &= \quad \sum_{n\,\text{odd}}\frac{1}{n!}\left(Ke^{-S_I/\hbar}\omega\tau\right)^n\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2} \\ &= \quad \sinh\left(Ke^{-S_I/\hbar}\omega\tau\right)\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2} \\ =-\frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}&\left(\exp\left\{-\left(\frac{1}{2}+Ke^{-S_I/\hbar}\right)\omega\tau\right\}-\exp\left\{-\left(\frac{1}{2}-Ke^{-S_I/\hbar}\right)\omega\tau\right\}\right) \qquad (7.21)\end{aligned}$$

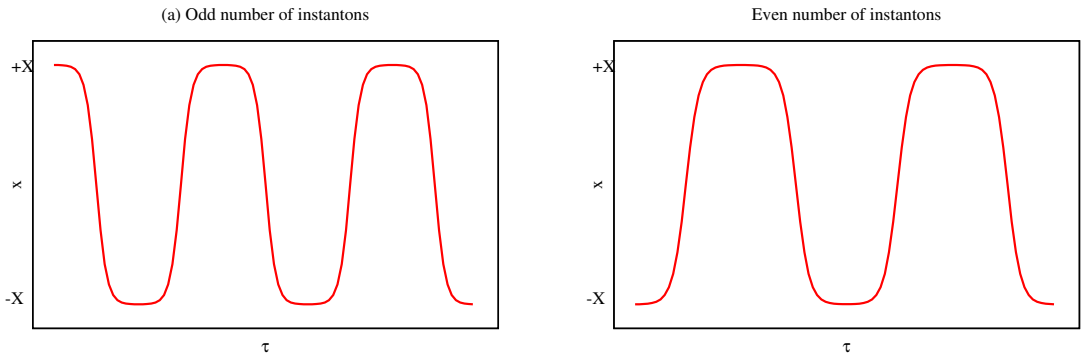

Figure 6: An example of an odd number of instantons (a), and an example of an even number of instantons

and summing over even n

$$\begin{aligned}\langle \pm\lambda, \frac{\tau}{2}\big| \mp \lambda, \frac{-\tau}{2}\rangle &= \sum_{n\,\text{even}} \frac{1}{n!}\left(Ke^{-S_I/\hbar}\omega\tau\right)^n \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2} \\ &= \cosh\left(Ke^{-S_I/\hbar}\omega\tau\right)\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2} \\ &= \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}\left(\exp\left\{-\left(\frac{1}{2}+Ke^{-S_I/\hbar}\right)\omega\tau\right\}+\exp\left\{-\left(\frac{1}{2}-Ke^{-S_I/\hbar}\right)\omega\tau\right\}\right) \quad (7.22)\end{aligned}$$

We see that the ground state energy is split into two levels with energies

$$E_+ = \left(\frac{1}{2}+Ke^{-S_I/\hbar}\right)\hbar\omega \quad (7.23)$$

and

$$E_- = \left(\frac{1}{2}-Ke^{-S_I/\hbar}\right)\hbar\omega. \quad (7.24)$$

The energy eigenstates are the superpositions of the states $\big|-\lambda\rangle$ and $\big|\lambda\rangle$

$$\big|E_+\rangle = \left(\frac{m\omega}{4\pi\hbar}\right)^{-1/4}\left(\big|\lambda\rangle - \big|-\lambda\rangle\right) \quad (7.25)$$

with a transition amplitude (in imaginary time) $\exp(-E_+\tau/\hbar)$ and

$$\big|E_-\rangle = \left(\frac{m\omega}{4\pi\hbar}\right)^{-1/4}\left(\big|\lambda\rangle + \big|-\lambda\rangle\right) \quad (7.26)$$

with a transition amplitude $\exp(-E_-\tau/\hbar)$.

7.4 Periodic Potentials

Consider a particle of mass m moving in a periodic potential such as

$$V(x) \;=\; m\left(\frac{\omega\lambda}{2\pi}\right)^2\left(1-\cos\left(\frac{2\pi x}{\lambda}\right)\right), \tag{7.27}$$

shown in Fig.7.

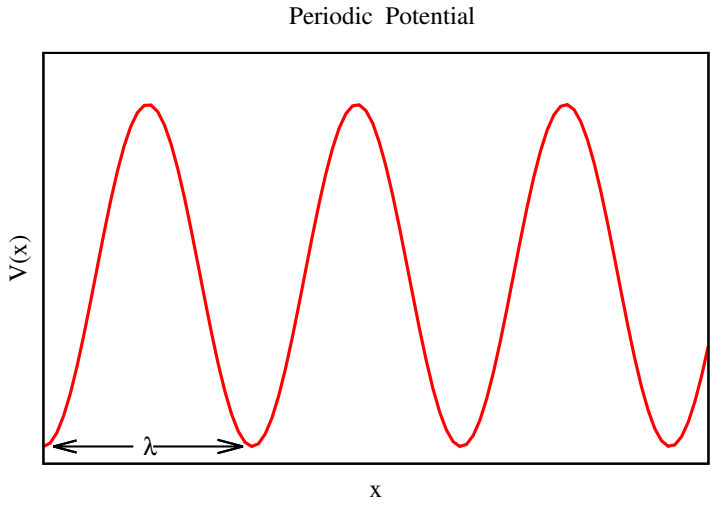

Figure 7: Periodic Potential

There are minima at $x = n\lambda$ for all integer n. Near these minima the potential may be approximated by

$$V(x) \;\approx\; \frac{1}{2}m\omega^2(x-n\lambda)^2.$$

Without the effect of instantons, which can effect transitions between adjacent minima, the system would have degenerate ground-states, each of which consisting of oscillations about one of the minima with ground-state energy $\frac{1}{2}\hbar\omega$. We denote these states by $|n\rangle$.

We can construct states which are linear superpositions of these states, denoted by a continuous parameter θ,

$$|\theta\rangle \;\equiv\; \sum_n e^{-in\theta}|n\rangle. \tag{7.28}$$

We will see that these states are energy eigenstates, with energy eigenvalues that depend on θ.

Quantum tunnelling between the minima is effected by an instanton path (in imaginary time $\tilde{\tau}$)

$$x_I(\tilde{\tau}) \;=\; \frac{2\lambda}{\pi}\tan^{-1}\left(e^{\omega(\tilde{\tau}-\tau_0}\right) \tag{7.29}$$

which is a solution to the sine-Gordon equation in one Euclidean dimension:

$$\frac{d^2}{d\tilde{\tau}^2}x_I(\tilde{\tau}) \;=\; \omega^2\lambda\sin\left(\frac{2\pi x_I(\tilde{\tau})}{\lambda}\right) \tag{7.30}$$

The action of this integral is

$$S_I \;=\; \frac{2m\omega\lambda^2}{\pi^2} \tag{7.31}$$

We note that x_I given by (7.29) varies from $n\lambda$ as $\tilde{\tau}\to-\infty$ to $(n+1)\lambda$ as $\tilde{\tau}\to+\infty$.

The anti-instanton path

$$\overline{x}_I(\tilde{\tau}) \;=\; x_I(-\tilde{\tau})$$

gives rise to transitions between $(n+1)\lambda$ as $\tilde{\tau}\to-\infty$ to $n\lambda$ as $\tilde{\tau}\to+\infty$.

As in the case of the double-well potential, the system possesses a zero mode

$$x_0(\tilde{\tau}) \;=\; \sqrt{\frac{m}{S_I}}\frac{d}{d\tau_c}x_{I_{\tau_c}}(\tilde{\tau}) \tag{7.32}$$

due to the fact that the centre of the instanton, τ_0, breaks the invariance under (imaginary-)time invariance and must be treated as a collective coordinate.

The amplitude for an instanton transition is given (in the semi-classical approximation) by

$$\langle(n+1),\frac{\tau}{2}|n,-\frac{\tau}{2}\rangle \;=\; Ke^{-S_I/\hbar}\omega\tau\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2}, \tag{7.33}$$

with S_I now given by (7.31) and the pre-factor K differs from that given by (7.12) by a numerical constant of order unity.

The transition amplitude between states $|n_1\rangle$ and $|n_2\rangle$ has contributions from l instantons and $\bar{l}$ anti-instantons, subject to the condition

$$l-\bar{l}=n_2-n_1$$

($\bar{l}$ instantons increases n by l and $\bar{l}$ instantons decreases n by $\bar{l}$).

Thus we have

$$\langle n_2,\frac{\tau}{2}|n_1,-\frac{\tau}{2}\rangle \;=\; \sum_{l,\bar{l}}\frac{1}{l!\bar{l}!}\left(Ke^{-S_I/\hbar}\omega\tau\right)^{(l+\bar{l})}\delta_{n_2-n_1-l+\bar{l}}\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2}, \tag{7.34}$$

Using the identity

$$\delta_{mn} \;=\; \frac{1}{2\pi}\int_0^{2\pi}e^{i(n-m)\theta}d\theta,$$

and performing the sum over $l,\bar{l}$ we get

$$\langle n_2,\frac{\tau}{2}|n_1,\frac{\tau}{2}\rangle \;=\; \frac{1}{2\pi}\int_0^{2\pi}d\theta e^{in_1\theta}e^{-in_2\theta}\exp\left\{Ke^{-S_I/\hbar}\omega\tau e^{i\theta}\right\}\exp\left\{Ke^{-S_I/\hbar}\omega\tau e^{-i\theta}\right\}\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2}, \tag{7.35}$$

Inverting (7.28)

$$|n\rangle \;=\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}|e^{in\theta}\rangle$$

and introducing $\delta(\theta-\theta')$, we end up with

$$\langle\theta',\frac{\tau}{2}|\theta,-\frac{\tau}{2}\rangle \;=\; \delta(\theta-\theta')\exp\left\{2Ke^{-S_I/\hbar}\omega\tau\cos\theta\right\}\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\omega\tau/2}. \tag{7.36}$$

The δ-function tells us that these θ states are energy eigenstates with energy

$$E(\theta) \;=\; \left(\frac{1}{2}-2Ke^{-S_I/\hbar}\cos\theta\right)\hbar\omega \tag{7.37}$$

8 Path Integrals in Quantum Field Theory

Henceforth we will adopt the system of units, normally used in particle physics, in which $\hbar=c=1$.

We have already seen how the path integral formalism in Quantum Physics can be applied to systems with several coordinates q_i (even though the examples considered were all one-dimensional).

The extension to quantum field theory is then straightforward, and can be understood immediately in the case where space is discredited with points $x_{\{j\}}$ and a field $\phi(x_{\{j\}},t)$ is a set of coordinates $\phi_{\{j\}}(t)$.

In the continuum limit for which the discrete space-like points

$$x_{\{j\}} \;\to \mathbf{x},$$

this large (infinite) set of discrete coordinates becomes a field ϕ,, which is a function of space $\mathbf{x}$ as well as time, t.

$$\phi_{\{j\}}(t) \;\to \phi(\mathbf{x},t).$$

The Lagrangian for a given field theory is expressed in terms of a (Lorentz invariant) Lagrangian density, $\mathcal{L}$:

$$L[\phi(\mathbf{x},t)] \;=\; \int d^3\mathbf{x}\mathcal{L}\left(\phi(\mathbf{x},t),\partial_\mu\phi(\mathbf{x},t)\right).$$

Note that since the Lagrangian generally depends on the field at neighbouring space-points, the Lagrangian density is a function of the spatial derivative of the field, $\boldsymbol{\partial}\phi$, as well as the time derivative.

Writing $\phi(\mathbf{x},t)$ as $\phi(x)$, where x_μ is the 4-vector $(\mathbf{x},t)$, the transition amplitude from an eigenstate of the field operator, with eigenvalue [6] $\phi_i(\mathbf{x})$ at time $t=-T/2$ to an eigenstate of the field operator, with eigenvalue $\phi_f(\mathbf{x})$ at time $t=+T/2$ is given by the path integral

$$\langle\phi_f(\mathbf{x}),T/2\big|\phi_i(\mathbf{x}),-T/2\rangle \;=\; \int \mathcal{D}(\phi(x))e^{iS[\phi(x]}, \tag{8.1}$$

where the $\mathcal{D}[\phi(x)]$, means integrate over all possible functions, $\phi(x)$ of space-time with boundary values

$$\phi(\mathbf{x},-T/2) \;=\; \phi(\mathbf{x})_i$$

and

$$\phi(\mathbf{x},+T/2) \;=\; \phi(\mathbf{x})_f$$

and the action $S[\phi(x)]$ is given by

$$S[\phi(x)] \;=\; \int_{-T/2}^{T/2} dt \int d^3\mathbf{x}\mathcal{L}(\phi(x),\partial_\mu\phi(x)) \tag{8.2}$$

More generally we have (in analogy with (4.3)

$$\begin{aligned}\langle\phi_f(\mathbf{x}),T/2\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|\phi_i(\mathbf{x}),-T/2\rangle \;&=\\ \int \mathcal{D}[\phi(x)]\phi(x_1)\phi(x_2)\cdots\phi(x_k)\exp\left(iS[\phi(x)]\right),&\end{aligned} \tag{8.3}$$

where $\hat{\phi}(x)$ is the quantum field operator at space-time point x.

The LHS of (8.3) can be expanded in terms of energy eigenstates $\big|E_n,\alpha\rangle$ (where α represents the set of quantum numbers for a member of the degenerate set of states with energy E_n).

$$\begin{aligned}&\langle\phi_f(\mathbf{x}),T/2\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|\phi_i(\mathbf{x}),-T/2\rangle \;=\\ &\sum_n\sum_\alpha \Psi^*_{n,\alpha}[\phi(\mathbf{x})_f]\Psi_{n,\alpha}[\phi(\mathbf{x})_i]\langle n,\alpha\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|n,\alpha\rangle e^{-iE_nT}\end{aligned} \tag{8.4}$$

where

$$\Psi_{n,\alpha}[\phi(\mathbf{x})_i] \;=\; \langle E_n\alpha\big|\phi_i(\mathbf{x})\rangle$$

is the wavefunctional of the state $\big|E_n,\alpha\rangle$ in terms of the field function $\phi(\mathbf{x})_i$. We will see that we do *not* need the explicit expressions for such wavefunctionals

Once again, this path integral is most conveniently calculated in imaginary time, effected by a Wick rotation $t\to -i\tilde{\tau}$. We can express the necessary results in real time by performing the reverse Wick rotation.

[6] The eigenvalues of the field operator are function of $\mathbf{x}$. Again this is more easily understood if we discrete space to a set of points $\mathbf{x}_j$ and consider the eigenstates of the field operator as the simultaneous eigenstate of the set of operators $\hat{\phi}(\mathbf{x}_j)$ with the set of eigenvalues $\phi(\mathbf{x}_j)$.

In imaginary time the action is transformed so that

$$S[\phi] \ \rightarrow iS_E[\phi],$$

where the Euclidean action, S_E is given by

$$S_E[\phi(x)] \ = \ \int_{-\tau/2}^{\tau/2} d\tilde{\tau} \int d^3\mathbf{x}\mathcal{L}(\phi(x), \partial_i\phi(x)),$$

where $i = 1 \cdots 4$ are now indices in 4-dimensional Euclidean space.

In the limit $\tau \rightarrow \infty$, the exponent on the RHS of (8.4) is now dominated by the lowest energy state (the vacuum state) $|0>$. In quantum field theory the fields are "normal ordered" so that the energy of the vacuum state is zero. Eq.(8.4) then becomes

$$\begin{aligned}\langle\phi_f(\mathbf{x}), \tau \rightarrow \infty\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|\phi_i(\mathbf{x}), \tau \rightarrow -\infty\rangle \ \ = \\ \Psi_0^*(\phi(\mathbf{x}_f)\Psi_0(\phi(\mathbf{x}_i)\langle 0\big|T\phi(x_1)\phi(x_2)\cdots\phi(x_k)\big|0\rangle \quad (8.5)\end{aligned}$$

Now using (8.3) and dividing both sides by the vacuum-state wavefunction, we have

$$\begin{aligned}\langle 0\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|0\rangle \ \ = \\ (\Psi_0^*(\phi(\mathbf{x}_f)\Psi_0(\phi(\mathbf{x}_i))^{-1}\int \mathcal{D}[\phi(x)]\phi(x_1)\phi(x_2)\cdots\phi(x_k)e^{-S_E[\phi(x)]} \quad (8.6)\end{aligned}$$

We do not need to know the vacuum-state wavefunctions because we can divide both sides by their corresponding expressions in the case $k = 0$ (no factors of the field multiplying the exponent in the path integral). This gives us

$$\frac{\langle 0\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|0\rangle}{\langle 0\big|0\rangle} \ = \ \int \mathcal{D}[\phi(x)]\phi(x_1)\phi(x_2)\cdots\phi(x_k)e^{-S_E[\phi(x)]} \quad (8.7)$$

or simply

$$\langle 0\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|0\rangle \ = \ \int \mathcal{D}[\phi(x)]\phi(x_1)\phi(x_2)\cdots\phi(x_k)e^{-S_E[\phi(x)]} \quad (8.8)$$

since $\langle 0\big|0\rangle = 1$. In the limit $\tau \rightarrow \infty$, $S_E[[\phi(x)]$ becomes simply

$$S_E[\phi(x)] \ = \ \int d^4x\mathcal{L}\left(\phi, \partial_i\phi(x)\right)$$

The correlators on the LHS of (8.8) are the Green's functions usually required in any Quantum Field Theory calculation. The RHS of (8.8) can be obtained in terms of functional derivatives with respect to a source function $j(x)$. The source function $j(x)$ is introduced by adding the terms

$$\int d^4x\, j(x)\phi(x)$$

to the action. We define the "generating functional" $Z[j]$ of the source function $j(x)$ as

$$Z[j] \equiv \int \mathcal{D}[\phi(x)] \exp\left(-S_E[\phi(x)] - \int d^4x j(x)\phi(x)\right) \tag{8.9}$$

and we have

$$\langle 0\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_k)\big|0\rangle = \frac{1}{Z[0]}\left(-\frac{\delta}{\delta j(x_1)}\right)\left(-\frac{\delta}{\delta j(x_2)}\right)\cdots\left(-\frac{\delta}{\delta j(x_k)}\right) Z[j]_{|j=0} \tag{8.10}$$

8.1 Propagators

The Lagrangian density contains terms quadratic in the field ϕ, which we may write as

$$\mathcal{L}_0 = \frac{1}{2}\phi(x)\hat{\mathcal{O}}\phi(x). \tag{8.11}$$

For a real scalar field (corresponding to a neutral spin-0 particle) after integrating

$$-\int d^4x \frac{1}{2}\left(\partial_i\phi(x)\right)^2$$

by parts, we find that (in Euclidean space) the operator $\hat{\mathcal{O}}$ is given by

$$\hat{\mathcal{O}} = \partial_i^2 - m^2 \tag{8.12}$$

In analogy with the technique used for calculating the path integral in the case of Quantum Mechanics, we perform the integral over all functions $\phi(x)$ by expanding $\phi(x)$ in terms of $\phi_n(x)$, the eigenfunctions [7] of $\hat{\mathcal{O}}$ with eigenvalues λ_n:

$$\phi(x) = \sum_{n=0}^{\infty} c_n\phi_n(x), \tag{8.13}$$

where

$$\hat{\mathcal{O}}\phi_n(x) = \lambda_n\phi_n(x).$$

The measure $\mathcal{D}[\phi(x)]$ is then written (up to an overall constant) as

$$\mathcal{D}[\phi(x)] = \prod_{n=0}^{\infty} dc_n.$$

We also expand the source function $j(x)$ as

$$j(x) = \sum_{n}^{\infty} j_n\phi_n(x)$$

[7] In an infinite volume there is a continuum of eigenfunctions and eigenvalues. This is most easily handled by assuming that the system is confined to a space-time box of length L and then finally setting L to infinity.

The path integral for $Z[j]_0$ is then

$$Z[j]_0 \;\propto\; \prod_{n=0}^{\infty} \exp\left\{-c_n^2 - j_n c_n\right\},$$

where the suffix 0 indicates that this applies to the part of the Lagrangian which is quadratic in the field, i.e. the free-particle Lagrangian.

We can perform the gaussian integral and we do not need to worry about the pre-factor involving $\det \hat{\mathcal{O}}$ because we are only interested in the dependence on the source as we are dividing the result by $Z[0]$ We therefore have

$$\frac{Z[j]_0}{Z[0]_{\,0}} \;=\; \prod_{n=0}^{\infty} \exp\left(\frac{j_n^2}{2\lambda_n}\right) \;=\; \exp\left\{\sum_{n=0}^{\infty} \frac{j_n^2}{2\lambda_n}\right\} \tag{8.14}$$

From the orthonormality of the eigenfunctions

$$j_n \;=\; \int d^4x j(x) \phi_n^*(x)$$

we may rewrite (8.14) as

$$\frac{Z[j]_0}{Z[0]_{\,0}} \;=\; \exp\left\{\int d^4x \int d^4y \frac{1}{2} j(x) \hat{\mathcal{O}}^{-1}(x,y) j(y)\right\} \tag{8.15}$$

In the case of a scalar particle

$$\hat{\mathcal{O}}^{-1}(x,y) \;=\; \int \frac{d^4k}{(2\pi)^4} e^{ik\cdot(x-y)} \frac{-1}{(k^2+m^2)}, \tag{8.16}$$

as can be checked by applying the operator $\hat{\mathcal{O}}$ to obtain

$$\int \frac{d^4k}{(2\pi)^4} e^{ik\cdot(x-y)} \;=\; \delta^4(x-y).$$

Note that by reversing the sign of the Fourier variable, k, in (8.16) we see that $\hat{\mathcal{O}}^{-1}(x,y)$ is symmetric under $x \leftrightarrow y$.

The two-point function (propagator) for a free particle is given by

$$\langle 0 \big| T\phi(x_1)\phi(x_2) \big| 0 \rangle_0 \;=\; \frac{-\delta}{\delta j(x_1)} \frac{-\delta}{\delta j(x_2)} Z[j]_0 \tag{8.17}$$

Since we are going to set $j(x) = 0$, we only need to expand the exponential in (8.15) up to second order in j and the functional derivatives give

$$\begin{aligned} \frac{-\delta}{\delta j(x_1)} \frac{-\delta}{\delta j(x_2)} \int d^4x d^4y \frac{1}{2} j(x) \hat{\mathcal{O}}^{-1}(x,y) j(y) \;&= \\ \int d^4x d^4y \frac{1}{2} \Big[\delta^4(x-x_1) \hat{\mathcal{O}}^{-1}(x,y) \delta^4(y-x_2) + \delta^4(x-x_2) \hat{\mathcal{O}}^{-1}(x,y) \delta^4(y-x_1)\Big] \\ &= \;\hat{\mathcal{O}}^{-1}(x_1,x_2) \end{aligned} \tag{8.18}$$

For a real scalar field we have the free propagator

$$\langle 0\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\big|0\rangle_0 \;=\; \int \frac{d^4k}{(2\pi)^4}e^{-ik\cdot(x-y)}\frac{-1}{(k^2+m^2)}, \tag{8.19}$$

We can perform the Wick rotation back to find the propagator in Minkowski space by setting $(x-y)_4$ to $i(x-y)_0$, which is equivalent to setting k_4 to $-ik_0$. However, we need to do this with care. The Fourier transform of the propagator contains poles at $k_4 = \pm i(\mathbf{k}^2+m^2)$, and we must not cross such poles when we perform a Wick rotation. The Wick rotation is therefore written more carefully as

$$k_0 = \lim_{\epsilon\to 0}\; \exp\left(-i\left(\frac{\pi}{2}-\epsilon\right)\right) k_4$$

and the propagator in Minkowski space is

$$\langle 0\big|T\hat{\phi}(x)\hat{\phi}(y)\big|0\rangle_0 \;=\; \lim_{\epsilon\to 0}\int \frac{d^4k}{(2\pi)^4}e^{-ik\cdot(x-y)}\frac{i}{(k^2-m^2+i\epsilon)} \tag{8.20}$$

We now return to Minkowski space for which the generating functional of the source $j(x)$ is

$$Z[j]_0 \;=\; Z[0]\exp\left\{-i\int d^4x\int d^4y\frac{1}{2}j(x)\hat{\mathcal{O}}^{-1}(x,y)j(y)\right\} \tag{8.21}$$

For the k-point Green function, (8.8) we see that since $Z[j]$ contains only even powers of j, the Green function vanishes if k is odd vanishes and for even $k=2l$ we consider the l^{th} term in the expansion of the exponential in (8.15) we have (in leading order)

$$\begin{aligned}\langle 0\big|T\hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_{2l})\big|0\rangle_0 \;&=\\ &\left(-i\frac{\delta}{\delta j(x_1)}\right)\left(-i\frac{\delta}{\delta j(x_2)}\right)\cdots\left(-i\frac{\delta}{\delta j(x_{2l})}\right)\left(\int d^4xd^4yj(x)\hat{\mathcal{O}}^{-1}(x,y)j(y)\right)^l\\ &= \sum_{\text{pairings}(i_kj_k)}\prod_{k=1}^{l}\langle 0\big|T\hat{\phi}(x_{i_k})\hat{\phi}_{j_k})\big|0\rangle_0\end{aligned} \tag{8.22}$$

This is the (vacuum expectation value of the) Wick contraction theorem.

In (8.20) we have the leading order propagator for a real scalar field. For a complex scalar field associated with a "charged" spin-0 particle we have

$$\langle 0\big|T\hat{\phi}(x)\hat{\phi}^*(y)\big|)\rangle_0 \;=\; \lim_{\epsilon\to 0}\int \frac{d^4k}{(2\pi)^4}e^{-ik\cdot(x-y)}\frac{i}{(k^2-m^2+i\epsilon)} \tag{8.23}$$

For a massive vectors field V^a_μ associated with a particle with spin-1 and a component a of some internal symmetry, the quadratic part of the Lagrangian density in Minkowski space (after integrating by parts) is

$$\frac{1}{2}V^a_\mu(x)\delta_{ab}\left[g^{\mu\nu}\left(\partial_\mu\partial^\mu+m^2\right)-\partial^\mu\partial^\nu\right]V^b_\nu(x)$$

The leading order propagator for such a vector field (in Minkowski space) is the inverse of the quadratic operator $\delta_{ab}\left[g^{\mu\nu}\left(\partial_\mu\partial^\mu + m^2\right) - \partial^\mu\partial^\nu\right]$ and we have

$$\langle 0\big|T\hat{V}^a_\mu(x)\hat{V}^b_\nu(y)\big|0\rangle_0 \;=\; \lim_{\epsilon\to 0}\delta_{ab}\int\frac{d^4k}{(2\pi)^4}e^{-ik\cdot(x-y)}\left(-g^{\mu\nu}+\frac{k^\mu k^\nu}{m^2}\right)\frac{i}{(k^2-m^2+i\epsilon)}. \quad (8.24)$$

8.2 Perturbation Theory

We now re-instate the interaction part of the Lagrangian density. Restricting ourselves for the moment to real scalar fields, the interaction Lagrangian density, $\mathcal{L}_I$, contains terms which are cubic or higher order in the field, $\phi(x)$. The action may be written

$$S[\phi(x)] \;=\; S_0[\phi(x)] + S_I[\phi(x)],$$

where

$$S_0 \;=\; \int d^4x\frac{1}{2}\phi(x)\hat{\mathcal{O}}\phi(x)$$

and

$$S_I \;=\; \int d^4x\mathcal{L}_I(\phi(x))$$

Provided the couplings (the coefficients of the powers of ϕ) in $\mathcal{L}_I$ are sufficiently small, we may expand the term $\exp(iS_I)$ so that the path integral may be expanded as

$$\int\mathcal{D}[\phi(x)]\phi(x_1)\phi(x_2)\cdots\phi(x_k)e^{iS[\phi]} \;=\; \sum_{n=0}^{\infty}\frac{1}{n!}\int\mathcal{D}[\phi(x)]\phi(x_1)\phi(x_2)\cdots\phi(x_k)\left(i\int d^4x\mathcal{L}_I(\phi(x)\right)^n e^{iS_0[\phi]} \quad (8.25)$$

Each term on the RHS of (8.25) is a Green's function (correlator) calculated in the approximation of keeping only the quadratic terms in the Lagrangian and given by (8.22).

We therefore have a perturbative expansion for any Green's function that we need to calculate up to a given order in the couplings that appear in the interaction Lagrangian.

8.3 Fermion Fields and Grassmann variables

The Dirac field $\Psi_\alpha(x)$, which carries a Dirac index, α, is associated with a spin-$\frac{1}{2}$ particle. The part of the Lagrangian density quadratic in the fields is

$$\mathcal{L}_0 \;=\; \overline{\Psi}^\beta(x)\hat{\mathcal{O}}^\alpha_\beta\Psi_\alpha(x)$$

where the Dirac matrix operator is given by

$$\hat{\mathcal{O}}^\alpha_\beta \;=\; (i\gamma^\mu\partial_\mu + m)^\alpha_\beta\,\Psi_\alpha(x).$$

Since a spin-$\frac{1}{2}$ particle obeys Fermi-Dirac statistics,the fields $\Psi(x)$ anti-commute.

To encode this the field $\Psi_\alpha(x)$ is expanded in terms of the eigenstates of $\hat{\mathcal{O}}^\alpha_\beta$

$$\hat{\mathcal{O}}^\alpha_\beta \psi_{\alpha,n}(x) \quad = \lambda_n \psi_{\beta,n}(x),$$

as

$$\Psi_\alpha(x) \;=\; \sum_{n=-1}^{\infty} c_n \psi_{\alpha,n}(x), \tag{8.26}$$

where the coefficients c_n are Grassmann variables with the following properties

1.
$$c_n c_m \;=\; -c_m c_n.$$

2.
$$\int c_n dc_n \;=\; 1.$$

3.
$$\int 1 dc_n \;=\; 0.$$

An immediate consequence of this is

$$e^{\lambda c_n} \;=\; 1 + \lambda c_n$$

and

$$\int dc_n e^{\lambda c_n} \;=\; \lambda.$$

The conjugate fields $\overline{\Psi}^\beta(x)$ is similarly expanded

$$\overline{\Psi}^\beta(x) \;=\; \sum_{n=-1}^{\infty} \overline{c}_n \overline{\psi}^\beta_n(x), \tag{8.27}$$

where $\overline{\psi}_n(x) = \psi_n(x)^\dagger \gamma^0$, and $\overline{c}_n$ are a further set of Grassmann variables (which also anti-commute with the Grassmann variables c_n)

In order to calculate the generating functional (suppressing the Dirac indices) $Z[j(x), \overline{j}(x)]$, we add to the action the source terms

$$\int d^4x \left(\overline{j}(x)\Psi(x) + \overline{\Psi}(x) j(x) \right),$$

where the sources $j(x), \overline{j}(x)$ are also anti-commuting and may be also be expanded in terms of the eigenstates, $\psi_n(x)$ of $\hat{\mathcal{O}}$:

$$\begin{aligned} j(x) &= \sum_{n=0}^{\infty} j_n \overline{\psi}_n(x) \\ \overline{j}(x) &= \sum_{n=0}^{\infty} \overline{j_n} \psi_n(x), \end{aligned}$$

where j_n and $\overline{j}_n$ are again Grassmann variables. Using the orthonormality relation

$$\int d^4x \psi_{\alpha,n}(x) \overline{\psi}^{\beta}_m(x) = \delta^{\beta}_{\alpha} \delta_{mn}$$

we can write

$$\int d^4x \left[\overline{\Psi}(x) \hat{\mathcal{O}} \Psi(x) + \overline{j}(x) \Psi(x) + \overline{\Psi}(x) j(x) \right] = \sum_{n=0}^{\infty} \left[\overline{c}_n \lambda_n c_n + \overline{j}_n c_n + \overline{c}_n j_n \right] \tag{8.28}$$

The measure of the path integral over all Dirac fields $\mathcal{D}[\Psi(x)]$ may be written (up to an overall constant)

$$\mathcal{D}[\Psi(x)] \mathcal{D}[\overline{\Psi}(x)] = \prod_{n=0}^{\infty} d\overline{c}_n dc_n$$

so that the generating functional

$$\begin{aligned} Z[j(x), \overline{j}(x)] &= \int \mathcal{D}[\overline{\Psi}(x)] \mathcal{D}[\Psi(x)] \exp\left\{ i \left(\overline{\Psi}(x) \hat{\mathcal{O}} \Psi(x) + \overline{j}(x) \Psi(x) + \overline{\Psi}(x) j(x) \right) \right\} \\ &= \prod_{n=0}^{\infty} d\overline{c}_n dc_n \exp\left\{ i \left(\overline{c}_n \lambda_n c_n + \overline{j}_n c_n + \overline{c}_n j_n \right) \right\} \end{aligned} \tag{8.29}$$

The integral over the Grassmann variables $\overline{c}_n, c_n$ are performed following the rules given in 1 and 2 above. This gives (up to an overall constant)

$$Z[j] = \prod_{n=1}^{\infty} i\lambda_n \left(1 + i\, \overline{j}_n \frac{1}{\lambda_n} j_n \right) \tag{8.30}$$

We may write

$$\prod_{n=1}^{\infty} i\lambda_n = \det(i\hat{\mathcal{O}})$$

and

$$\left(1 + i\overline{j}_n \frac{1}{\lambda_n} j_n \right) = \exp\left\{ i \int d^4x d^4y\, \overline{j}(x) \hat{\mathcal{O}}^{-1}(x,y) j(y) \right\}$$

and the (leading order) propagator is

$$\langle 0 \big| T \Psi(x_1) \overline{\Psi}(x_2) \big| 0 \rangle_0 = \lim_{\epsilon \to 0} i \int \frac{d^4k}{(2\pi)^4} e^{-ik\cdot(x-y)} \frac{(\gamma \cdot k + m)}{k^2 - m^2 + i\epsilon}. \tag{8.31}$$

We do not need to calculate the determinant of the operator $\hat{\mathcal{O}}$. We should note, however, that in the case of anti-commuting fields, this pre-factor comes in the numerator as opposed to the denominator as is the case when performing the path integral over fields associated with particles that obey Bose-Einstein statistics (and therefore commute).

One further consequence of the anti-commuting property of fermion fields is that the expression (8.22) for the vacuum expectation value of a string of fermion fields is modified to account for a sign change each time two fields are interchanged

$$\begin{aligned}\langle 0\big|T\hat{\Psi}(x_1)\hat{\overline{\Psi}}(x_2)\cdots\hat{\overline{\Psi}}(x_{2l})\big|0\rangle_0 \;\; &= \\ &\sum_{\text{pairings}(i_k j_k)} (-1)^{\text{p}} \prod_{k=1}^{l} \langle 0\big|T\hat{\Psi}(x_{i_k})\hat{\overline{\Psi}}(x)_{j_k})\big|0\rangle_0, \end{aligned} \tag{8.32}$$

where p counts the number of commutations of the fermion fields to arrange them in the order

$$\prod_{k=1}^{l} \Psi(x_{i_k})\overline{\Psi}(x_{j_k})$$

For example

$$\begin{aligned}\langle\big|T\hat{\Psi}(x_1)\hat{\overline{\Psi}}(x_2)\hat{\Psi}(x_3)\hat{\overline{\Psi}}(x_4)\big|0\rangle_0 \;\; &= \;\; \langle\big|T\hat{\Psi}(x_1)\hat{\overline{\Psi}}(x_2)\big|0\rangle_0\langle\big|T\hat{\Psi}(x_3)\hat{\overline{\Psi}}(x_4)\big|0\rangle_0 \\ &- \;\; \langle\big|T\hat{\Psi}(x_1)\hat{\overline{\Psi}}(x_4)\big|0\rangle_0\langle\big|T\hat{\Psi}(x_3)\hat{\overline{\Psi}}(x_2)\big|0\rangle_0. \end{aligned} \tag{8.33}$$

The negative sign in the second term arising because there are 3 interchanges in the transformation

$$\Psi(x_1)\overline{\Psi}(x_2)\Psi(x_3)\overline{\Psi}(x_4) \;\; \rightarrow \;\; \Psi(x_1)\overline{\Psi}(x_4)\Psi(x_3)\overline{\Psi}(x_2)$$

9 Gauge Fixing in Gauge theories

A gauge theory contains a set of massless vector bosons (gauge bosons), $A^a_\mu(x)$, which transform under global transformations as the adjoint representation of the gauge group, but under local transformations, $\Omega^a(x)$ they transform as

$$\mathbf{A}_\mu(x) \;\; \rightarrow \mathbf{A}_{\mathbf{\Omega},\mu}(x) \;\; = \;\; g\mathbf{\Omega}(x)^{-1}\mathbf{A}_\mu(x)\mathbf{\Omega}(x) + \mathbf{\Omega}(x)^{-1}\partial_\mu\mathbf{\Omega}(x), \tag{9.1}$$

where we have introduced the matrix notation

$$\mathbf{A}_\mu(x) \;\; \equiv \tau^a A^a_\mu(x), \quad \mathbf{\Omega}(x) \;\; \equiv \tau^a\Omega^a(x),$$

with τ^a being the generators of the Lie algebra in the defining representation, with normalisation $\text{Tr}(\tau^a\tau^b) = \frac{1}{2}\delta^{ab}$. For infinitesimal transformations for which we may approximate

$$\mathbf{\Omega}(x) \;\; \equiv \;\; e^{i\boldsymbol{\alpha}(x)} \;\; \approx \;\; \mathbb{1} + i\boldsymbol{\alpha}(x),$$

(9.1) becomes

$$\begin{aligned}\mathbf{A}_\mu(x) \;\rightarrow\; \mathbf{A}_{\boldsymbol{\alpha},\mu}(x) &= \mathbf{A}_\mu(x) + \partial_\mu \boldsymbol{\alpha}(x) + ig\left[\mathbf{A}_\mu(x), \boldsymbol{\alpha}(x)\right] \\ &= \mathbf{A}_\mu(x) + [\mathbf{D}_\mu, \boldsymbol{\alpha}] \end{aligned} \tag{9.2}$$

where the covariant derivative is defined (for a general representation of the gauge group) as

$$\mathbf{D}_\mu \;=\; \partial_\mu \mathbb{1} + ig\mathbf{A}^a_\mu,$$

where τ^a is the generator of the Lie algebra in the appropriate representation.

In terms of components, a, the change in the gauge field, δA^a_μ under an infinitesimal gauge transformation, $\boldsymbol{\alpha}$ is

$$\delta A^a_\mu \;=\; f^{abc} A^b_\mu \alpha^c + \frac{1}{g}\partial_\mu \alpha^a \tag{9.3}$$

We see from (8.24) that the propagator for a vector-particle is not defined in the massless limit. This is again due to a zero mode in the quadratic field operator.

To quadratic order the Lagrangian density for the gauge bosons may be written

$$\mathcal{L}_0 \;=\; \mathrm{Tr}\mathbf{A}_\mu(x)\hat{\mathbf{O}}^{\mu\nu}\mathbf{A}_\nu(x),$$

where the operator

$$\hat{\mathbf{O}}^{\mu\nu} \;=\; \left(-g^{\mu\nu}\partial^2 + \partial^\mu\partial^\nu\right)\mathbb{1} \tag{9.4}$$

This has a zero mode

$$\mathbf{A}_{\mu\,0}(x) \;=\; \partial_\nu \boldsymbol{\alpha}(x) \tag{9.5}$$

In analogy with the zero mode that was discussed in quantum mechanics in the presence of a classical solution which breaks a symmetry of the action, in the case of a gauge theory the vacuum solution $\mathbf{A}_\mu(x) = 0$, breaks the symmetry of the action under a gauge transformation, giving rise to a zero mode which is equal to the infinitesimal gauge transformation of $\mathbf{A}_\mu(x) = 0$. Using (9.2) we see that

$$\mathbf{A}_{\mu\,0}(x) \;= \delta_{\boldsymbol{\alpha}}(\mathbf{A}_\mu(x))_{\mathbf{A}_\nu(x)=0}. \tag{9.6}$$

The divergence of the vector-field propagator (8.24), in the limit $m \rightarrow 0$ arises because the path integral over all functions $\mathbf{A}(x)$ we multiply count paths which are related to each other by a gauge transformation, so that they generate the same value for the action.

$$S\left[\mathbf{A}_\mu(x)\right] \;=\; S\left[\mathbf{A}_{\boldsymbol{\Omega},\mu}(x)\right] \tag{9.7}$$

More precisely, when we expand the path $\mathbf{A}_\mu(x)$ in terms of eigenfuncitons $\mathbf{A}^n_\mu(x)$, of the operator $\hat{\mathbf{O}}^{\mu\nu}$, for each possible eigenvalue, λ_n there is an infinite number of eigenfunctions related to each other by

$$\mathbf{A}^n_\mu(x) \;\rightarrow \mathbf{A}^n_{\boldsymbol{\alpha},\mu}(x)$$

We eliminate the superfluous modes by taking only one eigenfunction for each eigenvalue, corresponding to the gauge $\boldsymbol{\alpha}(x) = 0$.

The generating functional of the source $\mathbf{j}^\mu(x)$ then becomes

$$Z\left[\mathbf{j}^\mu(x)\right] \;=\; \int D\left[\mathbf{A}_\mu(x)\right]\delta\left[\boldsymbol{\alpha}(x)\right]\exp\left\{i\int d^4x\left(\mathcal{L}\left(\mathbf{A}_\mu\right)+\mathrm{Tr}\{\mathbf{j}^\mu(x)\mathbf{A}_\mu(x)\}\right)\right\} \tag{9.8}$$

The δ-functional means a product of δ-functions for each point in space-time (x). It has a functional integral representation

$$\delta[f(x)] \;=\; \int \mathcal{D}[k(x)]\exp\left(2\pi i\int d^4x k(x)f(x)\right)$$

We need to specify what we mean by the gauge $\boldsymbol{\alpha}(x)=0$. We define this be requiring that the gauge field obeys some constraint

$$f\left(\mathbf{A}_\mu(x)\right)=0. \tag{9.9}$$

The choice of the function $f(\mathbf{A}_\mu(x))$ is called the "gauge choice" and the constraint (9.9) is called the "gauge condition".

The functional delta-functional $\delta[\boldsymbol{\alpha}(x)]$ may be replaced by the δ-functional $\delta\left[f(\mathbf{A}_\mu)\right]$, provided we also include a jacobian correspond to the change of arguments of the δ-functional. The path integral defining the generating functional then becomes

$$Z\left[\mathbf{j}^\mu(x)\right] \;=\; \int D\left[\mathbf{A}_\mu(x)\right]\mathcal{J}\delta\left[f\left(\boldsymbol{A}_\mu(x)\right)\right]\exp\left\{i\int d^4x\left(\mathcal{L}\left(\mathbf{A}_\mu\right)+\mathrm{Tr}\{\mathbf{j}^\mu(x)\mathbf{A}_\mu(x)\}\right)\right\}, \tag{9.10}$$

where the jacobian $\mathcal{J}$ is given by

$$\mathcal{J} \;=\; \det\left\{\frac{\delta}{\delta\boldsymbol{\alpha}|(x)}f\left(\mathbf{A}_{\boldsymbol{\alpha},\mu}(x)\right)|(\boldsymbol{\alpha}=0)\right\} \tag{9.11}$$

We discuss this jacobian in more detail in the next subsection. Meanwhile we return to the effect of imposing the constraint (9.9).

An example of $f(\mathbf{A}_\mu(x)=0$ is the axial gauge

$$n\cdot\mathbf{A}(x) \;=\; 0 \tag{9.12}$$

where n is any 4-vector (9.12) sets a component of the gauge field to zero. For such a gauge choice the propagator is (suppressing "$\lim''_{\epsilon\to 0}$)

$$\begin{aligned}\left\langle 0\middle|T\hat{\mathbf{A}}_\mu(x)\hat{\mathbf{A}}_\nu(y)\middle|0\right\rangle_0 \;&=\; \mathbb{1}\!\!\mathbb{1}\int\frac{d^4k}{(2\pi)^4}e^{-ik\cdot(x-y)}\left(-g^{\mu\nu}+\frac{(n^\mu k^\nu+k^\mu n^\nu)}{n\cdot k}-n\cdot n\frac{k^\mu k^\nu}{(n\cdot k)^2}\right)\\ &\qquad\frac{i}{(k^2+i\epsilon)}.\end{aligned} \tag{9.13}$$

We see by inspection that this propagator vanishes when contracted either with n_μ or n_ν.

Another often used gauge condition is the "Landau" gauge

$$\partial \cdot \mathbf{A}(x) = 0,$$

(which has the advantage of being Lorentz invariant - known as a "covariant gauge"). We can obtain the propagator in this case from (9.13) by replacing n^ν by k^ν to obtain

$$\langle 0 \big| T \hat{\mathbf{A}}_\mu(x) \hat{\mathbf{A}}_\nu(y) \big| 0 \rangle_0 \;=\; \mathbb{1} \int \frac{d^4k}{(2\pi)^4} e^{-ik\cdot(x-y)} \left(-g^{\mu\nu} + \frac{k^\mu k^\nu}{k^2} \right) \frac{i}{(k^2 + i\epsilon)}. \tag{9.14}$$

For other covariant gauges, such as the Feynman gauge, we need to use another trick. We impose the condition

$$\partial \cdot \mathbf{A} \;=\; \rho(x),$$

and then perform a weighted average by performing a functional integral over all function $\rho(x)$ with weight

$$\exp\left\{ i \int d^4x \frac{1}{2(1-\lambda)} \rho(x)^2 \right\} \tag{9.15}$$

This introduces an overall constant (i.e. independent of the gauge field) factor, which does not interest us as the Green's functions are obtained only form the functional derivatives of $\log\left(Z[j]\right]$ with respect to the sources. The generating functional in leading order is now given by

$$\begin{aligned} Z\left[\mathbf{j}^\mu(x)\right]_0 \;&=\; \int \mathcal{D}[\rho(x)] D\left[\mathbf{A}_\mu(x)\right] \mathcal{J} \delta\left[\partial \boldsymbol{A}_\mu(x) - \rho(x)\right] \\ &\exp\left\{ i \int d^4x \left(\frac{1}{2(1-\lambda)} \rho(x)^2 \;+ \mathrm{Tr}\{\mathbf{A}_\mu(x) \hat{\mathbf{O}}^{\mu\nu} \mathbf{A}_\nu(x)\} + \mathrm{Tr}\{\mathbf{j}^\mu(x)\; \mathbf{A}_\mu(x)\} \right) \right\} \end{aligned} \tag{9.16}$$

We perform the functional integral over the function $\rho(x)$ absorbing the δ-functional to get

$$\begin{aligned} Z\left[\mathbf{j}^\mu(x)\right]_0 \;&=\; \int \mathcal{D}\left[\mathbf{A}_\mu(x)\right] \mathcal{J} \\ &\exp\left\{ i \int d^4x \left(\frac{1}{2(1-\lambda)} (\partial \cdot \mathbf{A})^2 \;+ \mathrm{Tr}\{\mathbf{A}_\mu(x) \hat{\mathbf{O}}^{\mu\nu} \mathbf{A}_\nu(x)\} + \mathrm{Tr}\{\mathbf{j}^\mu(x) \cdot \mathbf{A}_\mu(x)\} \right) \right\} \end{aligned} \tag{9.17}$$

The new term in the exponent (after integration by parts) can be added to the term proportional to $\mathbf{A}_\mu \hat{\mathbf{O}}^{\mu\nu}\; \mathbf{A}_\nu$ to yield a modified operator

$$\hat{\mathbf{O}}'^{\mu\nu} \;=\; \left(-g^{\mu\nu}\partial^2 + \frac{\lambda}{(1-\lambda)} \partial^\mu \partial^\nu \right) \mathbb{1}$$

This modified operator *does* have a well-defined inverse and leads to a propagator

$$\langle 0 \big| T \hat{\mathbf{A}}_\mu(x) \hat{\mathbf{A}}_\nu(y) \big| 0 \rangle_0 \;=\; \mathbb{1} \int \frac{d^4k}{(2\pi)^4} e^{-ik\cdot(x-y)} \left(-g^{\mu\nu} + \lambda \frac{k^\mu k^\nu}{k^2} \right) \frac{i}{(k^2 + i\epsilon)}. \tag{9.18}$$

9.1 Faddeev-Popov ghosts

Now we consider the jacobian $\mathcal{J}$ in (9.17). This is the determinant of the derivative of the gauge condition with respect to an infinitesimal gauge transformation (9.3).

For an axial gauge we have (in components)

$$\mathcal{J} \ = \det n \cdot D^{ab} \ = \det \left(n.\partial \, \delta^{ab} - g f^{abc} n.A^c \right)$$

This is just

$$\mathcal{J} \ = \det n \cdot \mathbf{D} \ = \det n.\partial \, \mathbb{1},$$

since $n \cdot \mathbf{A} = 0$. This does not involve any fields and therefore it generates a constant factor, which cancels when the generating functional $Z[j^\mu]$ is divided by $Z[0]$.

For a covariant gauge (e.g. $\partial \cdot A^a = 0$) the jacobian is given by

$$\mathcal{J} \ = \ \det \left(\partial^2 \delta^{ab} - g f^{abc} A^c \cdot \partial \right)$$

In this case the jacobian *does* depend in the gauge field and needs to be handled appropriately.

The trick for doing so us to use the expression for the determinant of an operator expressed as an integral over Grassmann variables. To this end we fermion "fields" $\xi^a(x)$, $\eta^a(x)$ and we write

$$\mathcal{J} \ = \ \int \mathcal{D}[\xi(x)^a] \mathcal{D}[\eta^b(x)] \exp \left\{ \int d^4x \, \xi^a(x) \left(\partial^2 \delta^{ab} - g f^{abc} A^c \cdot \partial \right) \eta^b(x) \right\} \tag{9.19}$$

ξ^a and η^a look like fields but they do *not* correspond to any physical particle. They are known as "Faddeev-Popov ghosts". They carry no spin index, but they nevertheless obey Fermi-Dirac statistics. They transform as the adjoint representation of the gauge group (there is one for each gauge field).

These ghost fields never appear as external states, but they must be accounted for when considering loop corrections. They have the following properties

1. $\xi^a(x)$ propagates into $\eta^b(y)$ with a propagator for a massless scalar field

$$\langle 0 | T \xi^a(x) \eta^b(y) | 0 \rangle \ = \ \frac{i}{(2\pi)^4} \int d^4k e^{-ik \cdot (x-y)} \frac{\delta^{ab}}{(k^2 + i\epsilon)} \tag{9.20}$$

2. There is an interaction between ξ^a, η^b and the gauge field, A^c_μ with Feynman rule

$$g f^{abc} p_\mu,$$

   where p_μ is the outgoing momentum of η^b

3. There is a factor of (-1) for each loop of Faddeev-Popov ghosts due to the fact that they obey Fermi-Dirac statistics.

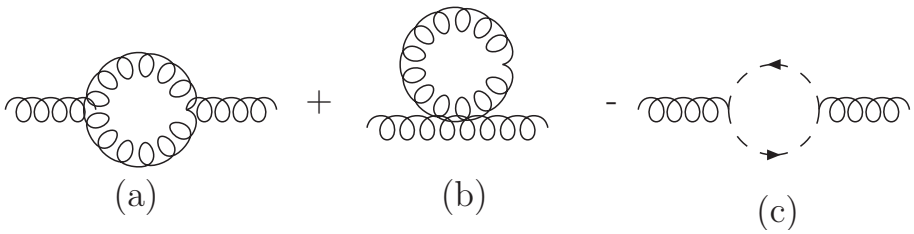

Figure 8: Instanton path. One-loop self-energy diagrams for a pure gauge field. Graph (c) is the contribution from the Faddeev-Popov ghosts. It carries a factor of (-1) since the ghost particles obey Fermi-Dirac statistics, The arrow indicated propagation from ξ to η.

An example is shown in Fig.8 for the one-loop self-energy of a gauge particle.

The existence of Faddeev-Popov ghosts can be inferred from unitarity considerations. The imaginary part of graph(a) is related by the Optical Theorem to the cross-section for the production of on-shell gauge particles. However, an on-shell vector-particle has three degrees of polarisation, whereas a gauge-boson only has two (one being eliminated by the choice of gauge). The Faddev-Popov graph with its negative sign serves to cancel the contribution from the superfluous degree of freedom in the cut graph (a).

10 Instantons in Gauge Theories

10.1 Topological Vacua

The gauge choice discussed above is not sufficient to determine the gauge field uniquely. A vacuum state can be any state in which the gauge field takes a value given by a pure gauge transformation acting of $\mathbf{A}_\mu \equiv 0$, namely

$$\mathbf{A}^{\mathbf{\Omega}}_\mu(x) \;=\; \frac{1}{g}\mathbf{\Omega}^{-1}(x)\partial_\mu\mathbf{\Omega}(x). \tag{10.1}$$

$\mathbf{\Omega}(x)$ maps the gauge group $\mathcal{G}$ to space-time. Suppose that at a particular time we have a vacuum state. The spatial coordinates of the gauge field, which obey the boundary condition that they vanish at spatial infinity, are given by

$$\mathbf{A}^{\mathbf{\Omega}}_i(\mathbf{x}) \;=\; \frac{1}{g}\mathbf{\Omega}^{-1}(\mathbf{x})\partial_i\mathbf{\Omega}(\mathbf{x}), \tag{10.2}$$

where

$$\mathbf{\Omega}(\mathbf{x}) \;\stackrel{|\mathbf{x}|\to\infty}{\longrightarrow}\; \mathbb{1}.$$

Since all the points on the boundary of space, R_3, are mapped to the identity element of the gauge group, we are actually mapping the gauge group onto the three-sphere, S_3 - which is the three-dimensional space, R_3, with all the points at infinite $|\mathbf{x}|$ identified.

If the gauge group is $SU(2)$ or contains an $SU(2)$ subgroup, this is a map from S_3 to S_3, since S_3 is the space of the group $SO(3)$, which is homomorphic to $SU(2)$ (two elements of $SU(2)$ can be mapped to each element of $SO(3)$). Such mappings can be classified into "homotopy classes" which determine the number of times the group space is "wrapped" around the spatial S_3. For the homotopy class $n = 0$, the mapping does not wrap around the space at all and can be continuously deformed to the trivial map

$$\mathbf{\Omega}(\mathbf{x}) \equiv \mathbb{1},$$

In other words, a map in the homotopic class zero can be constructed from a large number of infinitesimal gauge transformations with infinitesimal parameter $\boldsymbol{\alpha}(\mathbf{x})$, with boundary condition

$$\boldsymbol{\alpha}(|\mathbf{x}| \to \infty) \;=\; \mathbf{0},$$

i.e.

$$\mathbf{\Omega}_{n=0}(\mathbf{x}) \;=\; \lim_{N\to\infty, |\boldsymbol{\alpha}|\to 0} (\mathbb{1} + i\boldsymbol{\alpha}(\mathbf{x}))^N$$

However, for the non-zero homotopy classes this is not possible. On the other hand, all mappings within a given class can be transformed into each other by a continuous gauge transformation.

The gauge choice selects one vacuum state for each homotopy class, but the vacuum is still degenerate, with a quantum number corresponding to the homotopy class of the mapping.

10.1.1 One dimensional example

This concept is more easily understood in a simple example of the gauge group $U(1)$ in one space dimension.

If the gauge transformation is the identity at $x = \pm\infty$, then we identify the two ends of the line to obtain a circle – a one-dimensional spherical surface S_1 – with coordinate θ in the range

$$0 \;<\; \theta \leq\; 2\pi.$$

The group mapping is given by

$$\Omega(\theta) \;=\; e^{if(\theta)}.$$

Since Ω has to be single-valued we require

$$f(\theta + 2\pi) \;= f(\theta),$$

so that the most general form of $U(\theta)$ has phase

$$f(\theta) \;= n\theta + h(\theta),$$

where n is an integer and the function $h(\theta)$ obeys the boundary conditions

$$h(0) \;=\; h(2\pi) \;= 0$$

As θ increases from 0 to 2π the $U(1)$ phase increases from zero to $2n\pi$ - the group is "wrapped" around spatial S_1 n times.

For $n = 0$ we can write

$$\Omega(\theta) \;=\; \lim_{N\to\infty}\left(1 + i\frac{1}{N}h(\theta)\right)^N,$$

but for $n \neq 0$ this is not possible.

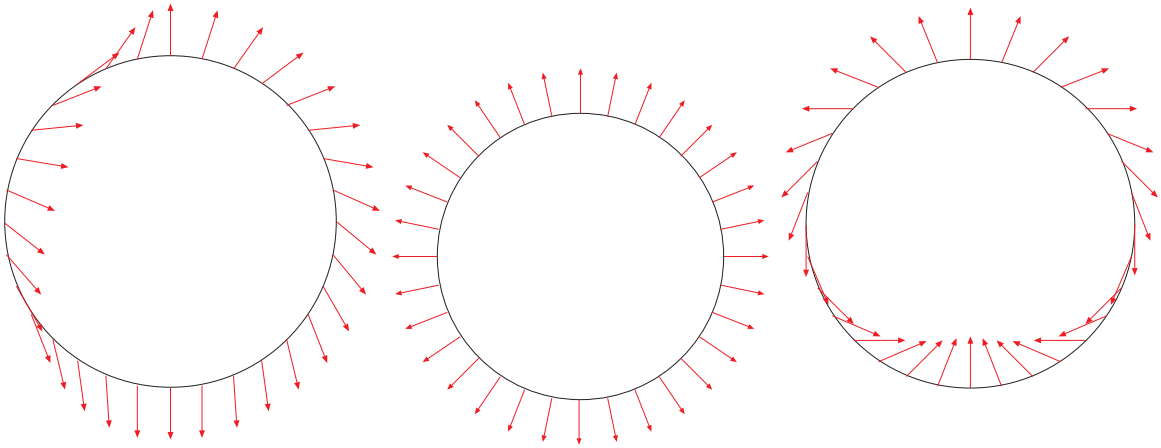

Figure 9: Examples of $U(1)$ maps with different homotopies. The phase of the element of $U1)$ is the angle of orientation of the arrow at a given point on the circle, relative to the upward vertical.
(a) represents a mapping in the homotopy class $n = 0$. An anti-clockwise rotation of the arrows through an angle which increases from zero at the top to π at the bottom can bring all the arrows into the vertically upward state – representing the trivial map in which all points on the circle are mapped to the identity element of $U(1)$.
(b) is an example of a map of homotopy class $n = 1$. We see that any attempt to rotate all of the arrows so that they are pointing vertically upwards will generate a discontinuity somewhere. As one moves around the circle from zero to 2π the arrow also rotates through a complete circle.
(c) is an example of a map in the homotopy class $n = 2$. As one moves around the circle, the arrow makes two complete rotations.

The corresponding gauge field $A(\theta)$ is given by

$$A(\theta) \;=\; \frac{1}{g}\Omega^{-1}(\theta)\partial_\theta\Omega(\theta) \;= \frac{1}{g}\left(n + h'(\theta)\right))$$

The homotopy class or "winding number" n can be obtained as an integral over the gauge field

$$n \;=\; \frac{g}{2\pi}\int d\theta A(\theta), \tag{10.3}$$

where we have made use of the boundary values of the function $h(\theta)$.

A gauge condition such as $\partial_\theta A(\theta) = 0$ only specifies the gauge field up to the addition of an integer.

10.1.2 Chern-Simon form

In three space-dimensions, the mapping of the gauge manifold for the group $SU(2)$ onto the space S_3 also has homotopy classes which specify the number of times n that the group manifold S_3/Z_2 covers the S_3 space. Once again, a gauge specifies one unique vacuum gauge field (as a function of $\mathbf{x}$) for *each* winding number n.

An example of a gauge transformation in homotopy class $n = 1$ is

$$\mathbf{U}_{n=1} \ = \exp\left\{-i\pi \frac{x_i \tau^i}{|\mathbf{x}|^2 + \rho^2}\right\} \tag{10.4}$$

In terms of the vacuum gauge-field $\mathbf{A}_i^{\mathbf{\Omega}}(\mathbf{x})$, the winding number n is given by

$$n \ = \ \int d^3\mathbf{x} K_0(x)$$

where K_0 is called the "Chern-Simons three form" and is given by

$$K_0 \ = \ \frac{g^2}{8\pi^2}\epsilon_{ijk}\mathrm{Tr}\left\{\mathbf{A}_i \partial_j \mathbf{A}_k + \frac{2ig}{3}\left[\mathbf{A}_i, \mathbf{A}_j\right]\mathbf{A}_K\right\} \tag{10.5}$$

10.1.3 θ-vacua

In analogy with the case of a periodic potential for a quantum mechanical system, we can define states parameterised by an angle θ, which are superpositions of the degenerate states labelled by winding number n.

$$|\theta\rangle \ = \ \sum_n e^{-in\theta}|n\rangle.$$

We will see that there are instantons which can affect tunnelling between vacua with different winding number n and that this tunnelling splits the degeneracy of the states with different values of θ.

10.2 Instantons in a Pure Gauge Theory

We now investigate the existence of gauge-field configurations (gauge theory instantons) which can affect tunnelling between vacua with different winding number n, in other words

$$\Delta n \ \equiv n(t \to +\infty) - n(t \to -\infty) \neq 0.$$

We now consider the gauge field to depend on time as well as space, and only for very early or very late times, $t \to \mp\infty$ is the gauge field a vacuum configuration

$$\mathbf{A}_\mu(\mathbf{x}, t = \pm\infty) \;=\; \mathbf{\Omega}^{-1}(\mathbf{x})\partial_\mu\mathbf{\Omega}(\mathbf{x}).$$

$$\Delta n \;= \left(\int d^3\mathbf{x} K_0(\mathbf{x}, t \to +\infty) - \int d^3\mathbf{x} K_0(\mathbf{x}, t \to -\infty)\right) \tag{10.6}$$

We can consider the Chern-Simons three-form K_0 to be the zero-component of the four-vector

$$K_\mu \;\equiv \frac{g^2}{8\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}\left\{\mathbf{A}^\nu\partial^\rho\mathbf{A}^\sigma + \frac{2ig}{3}\left[\mathbf{A}^\nu, \mathbf{A}^\rho\right]\mathbf{A}^\sigma\right\}, \tag{10.7}$$

where the gauge fields are now taken to be functions of space-time, x. Using Gauss' theorem we can then write

$$\Delta n \;=\; \int d^4x\, \partial^\mu K_\mu(x) \tag{10.8}$$

Taking the divergence of K_μ defined in (10.7) We find

$$\partial^\mu K_\mu \;=\; \frac{1}{2}\mathrm{Tr}\{\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\}, \tag{10.9}$$

where

$$\tilde{\mathbf{F}}_{\mu\nu} \equiv\; \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}\mathbf{F}^{\rho\sigma},$$

is the dual of the field strength

$$\mathbf{F}_{\mu\nu} \;\equiv\; \partial_\mu\mathbf{A}_\nu - \partial_\nu\mathbf{A}_\mu + ig\left[\mathbf{A}_\mu, \mathbf{A}_\nu\right].$$

(10.8) and (10.9) then give us

$$\Delta n \;=\; \frac{g^2}{16\pi^2}\int d^4x\mathrm{Tr}\left\{\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\right\} \tag{10.10}$$

For the case of the θ vacua, the existence of such an instanton which can affect a change of homotopy class by Δn is equivalent to adding a term

$$\delta S[\mathbf{A}] \;\equiv \frac{g^2}{16\pi^2}\int d^4x\mathrm{Tr}\{\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\}$$

to the action. We see that a transition from a vacuum in homotopy class n_1 at early time, $-\frac{1}{2}\tau$ to a vacuum in homotopy class n_2 at late time, $+\frac{1}{2}\tau$, is given by

$$\langle n_2, \frac{1}{2}\tau | n_1, -\frac{1}{2}\tau\rangle \;\sim\; e^{-S[\mathbf{A}]}\delta_{(n_1-n_2),\Delta n},$$

where we are not worrying about the pre-factor. For θ vacua, we have

$$\begin{aligned}\langle\theta, \frac{1}{2}\tau|\theta', -\frac{1}{2}\tau\rangle &\sim \sum_{n_1,n_2} \exp\left\{\frac{(n_1+n_2)}{2}(\theta-\theta')\right\}\exp\left\{\frac{(n_1-n_2)}{2}(\theta+\theta')\right\} e^{-S[\mathbf{A}]}\delta_{(n_2-n_1),\Delta n} \\ &= \delta(\theta-\theta')\exp\{-S[\mathbf{A}]-\theta\Delta n\} \\ &= \exp\left\{-S[\mathbf{A}]-\theta\int d^4x\frac{g^2}{16\pi^2}\mathrm{Tr}\{\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\}\right\} \qquad (10.11)\end{aligned}$$

Now from the inequality

$$\int d^4x \left|\mathbf{F}_{\mu\nu} - \tilde{\mathbf{F}}_{\mu\nu}\right|^2 \;\geq\; 0$$

This inequality may be written in terms of the Euclidean-space action, $S_E[\mathbf{A}]$, for a pure gauge theory as

$$S_E[\mathbf{A}] \;\equiv\; \frac{1}{2}\int d^4x \mathrm{Tr}\{\mathbf{F}^{\mu\nu}\cdot\mathbf{F}_{\mu\nu}\} \;\geq\; \frac{1}{2}\int d^4x \mathrm{Tr}\{\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\}. \qquad (10.12)$$

or

$$\frac{g^2}{8\pi^2}S[\mathbf{A}] \;\geq\; \Delta n. \qquad (10.13)$$

Therefore, if we can find a gauge-field configuration, $\mathbf{A}_I(x)$, (in Euclidean space) for which the index (10.10) (known as the "Pontryagin index") is non-zero, then there will be a minimum of the action subject to that value of the Pontryagin index, and therefore a solution of the classical equation of motion in Euclidean space. For such minimum the inequality (10.12) is saturated and the gauge-field configuration $\mathbf{A}_{I\mu}$, is "self-dual", i.e.

$$\mathbf{F}_{\mu\nu} \;=\; \tilde{\mathbf{F}}_{\mu\nu}$$

This gauge configuration is an instanton which affects a transition between two vacua whose homotopic class differs by Δn. Once again, in Minkowski space this is a space-time gauge-field configuration which corresponds to vacua in different homotopic classes at very early and very late times, but it is *not* a solution of the classical equations of motion in Minkowski space and therefore is not interpreted as a particle.

An anti-instanton, which affects a transition between two vacua whose homotopy class differ by $-\Delta n$ is anti-self-dual, i.e.

$$\mathbf{F}_{\mu\nu} \;=\; -\tilde{\mathbf{F}}_{\mu\nu}$$

In the case $\Delta n = 1$, the instanton gauge field configuration is given by

$$A^a_{I\mu} \;=\; \frac{2}{g}\overline{\eta}_{a\mu\nu}\frac{\rho^2(x-x_0))^\nu}{\left((x-x_0)^2+\rho^2\right)}, \qquad (10.14)$$

where the "t.Hooft symbols", $\overline{\eta}$ are given by

$$\begin{aligned}
\overline{\eta}_{aij} &= \epsilon_{aij},\ (i,j=1\cdots 3)\\
\overline{\eta}_{ai4} &= \delta_{ai}\\
\overline{\eta}_{a4i} &= -\delta_{ai}\\
\overline{\eta}_{a44} &= 0
\end{aligned} \tag{10.15}$$

Explicit calculation shows that (in Euclidean space)

$$\mathbf{F}_I^{\mu\nu} \;=\; \tilde{\mathbf{F}}_I^{\mu\nu}$$

and that the action

$$S[\mathbf{A}_I] \;=\; \frac{8\pi^2}{g^2} \tag{10.16}$$

so that the Pontryagin number

$$\Delta n \;=\; 1,$$

meaning that in Minkowski space this instanton gauge-field configuration affects a transition between a vacuum state in homotopy class n to a vacuum state in homotopy class $(n+1)$.

Note that for large (Euclidean) x^μ the instanton field is a pure gauge

$$\mathbf{A}_I^\mu(x) \stackrel{|x|\to\infty}{\longrightarrow} \mathbf{U}_I^{-1}(x)\partial^\mu \mathbf{U}_I(x),$$

where

$$\mathbf{U}_I(x) \;=\; \frac{x_4 \mathbb{1} + \tau^i x_i}{|x|}$$

The expression (10.14) for the instanton gauge-field is in a particular gauge, namely

$$x\cdot \mathbf{A}_I \;= 0.$$

This is the "singular gauge" since it is not defined at the origin.

A gauge transformation, $\mathbf{V}(x)$, exists which can transform this into a more commonly used gauge such as the axial gauge $\mathbf{A}_I^0 = 0$. The gauge transformation $\mathbf{V}$ is rather complicated but has the property

$$\mathbf{V}(x_4 \to +\infty, \mathbf{x}) = \mathbf{U}_{n=1}(\mathbf{x})\cdot \mathbf{V}(x_4 \to -\infty, \mathbf{x}),$$

where $\mathbf{U}_{n=1}$ is the homotopy class $n=1$ gauge transformation on S_3 given in (10.4). This shows explicitly how an instanton tunnels between vacua in adjacent homotopy classes.

10.2.1 Zero Modes and Collective Coordinates

The instanton (10.14) depends on the parameters x_0^μ, which determine the centre of the instanton and ρ, which determines its size.

Specifying these quantities breaks the invariance of the (Euclidean) action under (four-dimensional) translations

$$x^\mu \ \rightarrow \ x^\mu + x_0^\mu$$

and dilations

$$x^\mu \ \rightarrow \rho x^\mu; \ \mathbf{A}_\mu \ \rightarrow \frac{1}{\rho}\mathbf{A}_\mu$$

We therefore have 5 zero modes which are exchanged for the collective coordinates x_0^μ and ρ, each one introducing a jacobian factor of $\sqrt{S[\mathbf{A}_I]}$.

There are three further zero-modes associated with the breaking a rotational invariance and global $SU(2)$ invariance. There are only three such zero modes, since it turns out that the instanton configuration (10.14) is invariant under a linear combination of an infinitesimal rotation in space and an infinitesimal global SU(2) transformation. These three zero modes are exchanged for three angles of rotation (in a combined configuration space and internal $SU(2)$ space)[8]

The jacobian for this exchange between these zero modes and collective coordinates again carries a factor of $\sqrt{S[\mathbf{A}_I]}$. each and additionally a factor of ρ for each rotational zero-mode, which is required to compensate for the dimensional difference between an angle and a spatial coordinate (or size).

The amplitude for transition from a vacuum in homotopy class n to a vacuum in homotopy class $(N+1)$ (in Euclidean space) is then given by (using (10.16))

$$\langle (n+1), \tau \rightarrow +\infty | n, \tau \rightarrow -\infty \rangle_I \ = K \ \int d^4x_0 \int \frac{d\rho}{\rho^5} \left(\frac{8\pi^2}{g^2}\right)^4 \exp\left\{-\frac{8\pi^2}{g^2}\right\}, \qquad (10.17)$$

for the product of the non-zero eigenvalues of the quadratic operator in the presence of an instanton (divided by the determinant of the quadratic operator in zero background field).

Let us write this as

$$\langle (n+1)|n\rangle_I \ = \langle 0 \left| \exp\left\{ i \int d^4x \mathcal{L}_I(x) \right\} \right| 0 \rangle, \qquad (10.18)$$

where $\mathcal{L}_I$ is the effective Lagrangian density due to the instanton, to leading order in by

$$\mathcal{L}_I \ = \ \int \frac{d\rho}{\rho^5} \left(\frac{8\pi^2}{g^2}\right)^4 \exp\left\{-\frac{8\pi^2}{g^2}\right\}, \qquad (10.19)$$

[8]In the case of a gauge group which is larger than $SU(2)$ but has an $SU(2)$ subgroup, there are more zero modes, since there are more generators of the global gauge group which are broken by the instanton configuration. For an $SU(N)$ gauge group there are $4N-5$ rotational zero modes.

The integral over the instanton size is regulated as $\rho \to 0$ by the fact that the gauge coupling,. g should be integrated as the running coupling at scale $1/\rho$ so that (10.19) should read

$$\mathcal{L}_I \;=\; K \int \frac{d\rho}{\rho^5} \left(\frac{8\pi^2}{g^2(1/\rho)} \right)^4 \exp\left\{ -\frac{8\pi^2}{g^2(1/\rho)} \right\}, . \tag{10.20}$$

For sufficiently small ρ and for a $SU(2)$ pure gauge theory

$$\exp\left\{ -\frac{8\pi^2}{g^2(1/\rho)} \right\} \;\sim \rho^{22/3},$$

so that the $\rho \to 0$ limit is regularised even if we add (not too many) generations of fermions.

For large ρ the coupling becomes last and perturbation theory is unreliable. It is expected that for these large values of the gauge coupling, non-perturbative effects attenuate the integrand over ρ so tha that maximum size of ρ is of order $1/\Lambda_{\rm QCD}$.

As in the case of the periodic potential, we now need to sum over all sequences of instantons and anti-instantons and the upshot is that the effective Lagrangian density density, of the θ-vacua acquire and extra term

$$\Delta\mathcal{L}(\theta) \propto -\int \frac{d\rho}{\rho^5} \left(\frac{8\pi^2}{g^2(1/\rho)} \right)^4 \exp\left\{ -\frac{8\pi^2}{g^2(1/\rho)} \right\} \cos\theta. \tag{10.21}$$

10.3 Axial Anomaly

If we include N massless fermions, $\Psi(x)$, which transform in the defining representation of an $SU(N)$ gauge theory then the Lagrangian is invariant under a chiral transformation in which *both* the left-handed and right-handed fermions transform separately under a global $U(N)$:

$$\begin{aligned} \Psi_L \;&\to\; e^{i\tau^a \alpha_L^a} \Psi_L \\ \Psi_R \;&\to\; e^{i\tau^a \alpha_L^a} \Psi_R, \end{aligned}$$

where the τ^a are the generators of $SU(N)$ supplemented by the identity, so as to promote the $SU(N)$ invariance to a $U(1)$ invariance for both the left-handed and right-handed fermions. In QCD only the vector $SU(N)$ for which $\alpha^a = \frac{1}{2}\left(\alpha_L^a + \alpha_R^a\right)$, is gauged (i.e. this combination of transformation parameters is a function of x).

In the absence of a mass term for the fermions there exists both a global vector $U(1)$ and a global axial $U(1)$

$$\begin{aligned} \Psi \;&\to e^{i\alpha_V} \Psi, \quad \text{and } \overline{\Psi} \;\to\; \overline{\Psi} e^{-i\alpha_V} \\ \Psi - \;&\to\; e^{i\gamma^5 \alpha_A} \Psi \;\text{ and } \overline{\Psi} \;\to\; \overline{\Psi} e^{i\alpha_A \gamma^5}, \end{aligned}$$

under which the Lagrangian is invariant.

One might have expected that since the Lagrangian is invariant under this axial $U(1)$ transformation, i.e. all Green's functions resulting from such a Lagrangian to be also invariant under axial transformations.

Unfortunately, this is *not* the case and the reason is that Quantum Field theories are subject to ultraviolet divergences which have to be regulated. It turns out that it is often impossible to construct a regulator which respects all of the symmetries of the original Lagrangian. Axial $U(1)$ is an example of one such invariance which is broken by the introduction of a gauge-invariant regulator.

In terms of path-integrals the generating functional for a gauge theory with massless fermions is a functional of the fermions sources $\overline{\eta}(x)$, $\eta(x)$ and the gauge-field source $\mathbf{j}_\mu(x)$

$$\begin{aligned} Z\left[\overline{\eta},\eta,\mathbf{j}_\mu\right] &= \int \mathcal{D}[\overline{\Psi}]\mathcal{D}[\Psi]\mathcal{D}'[\mathbf{A}_\mu] \\ &\times \exp\left\{ i\int d^4x \left(-\frac{1}{2}\mathrm{Tr}\{\mathbf{F}^{\mu\nu}\mathbf{F}_{\mu\nu}\} + i\overline{\Psi}\not{\mathbf{D}}\psi + \overline{\Psi}\eta + \overline{\eta}\Psi + \mathrm{Tr}\{\mathbf{j}\cdot\mathbf{A}\}\right)\right\} \end{aligned} \tag{10.22}$$

where the covariant derivative,

$$\mathbf{D}_\mu \equiv \partial_\mu \mathbb{1} + ig\mathbf{A}_\mu,$$

(and for the path integral over the gauge-field $\mathcal{D}'$ means integrate over all paths subject to a given gauge choice and Faddeev-Popov term where appropriate.)

Under an axial $U(1)$ transformation the action is invariant, but the fermion path integral measure $\mathcal{D}[\overline{\Psi}]\mathcal{D}[\Psi]$ acquires a jacobian from the transformation. This jacobian turns out to be ultra-violet divergent and needs to be regulated in a gauge invariant way. This regulator leads to a generating functional, $Z[\overline{\eta},\eta,\mathbf{j}_\mu]$, which has an (anomalous) variation under an infinitesimal axial $U(1)$ transformation with parameter, $\delta\alpha$.

$$\delta \log Z[\overline{\eta},\eta,\mathbf{j}_\mu] = \delta\alpha \frac{g^2}{8\pi^2}\int d^4x \mathrm{Tr}\{\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\} \tag{10.23}$$

The clearest way to see this is to calculate explicitly the divergence of the matrix element of the $U(1)$ axial current,

$$j^5_\mu(x) \equiv \overline{\Psi}(x)\gamma_\mu\gamma^5\Psi(x), \tag{10.24}$$

between the vacuum and a state consisting of two on-shell (massless) gauge-bosons with momenta p_1, p_2, colours a, b, and polarisation vectors ϵ_1, ϵ_2,

$$\partial^\mu \langle p_1,\epsilon_1,a;p_2,\epsilon_2,b|j^5_\mu(x)|0\rangle$$

If it were not for the anomaly, this would vanish, since if axial $U(1)$ symmetry is strictly obeyed the axial current is conserved - its divergence vanishes.

If there is an anomaly in the axial current then the divergent of the axial current couples to the two gauge-boson state via triangular fermion loops shown in Fig.10.

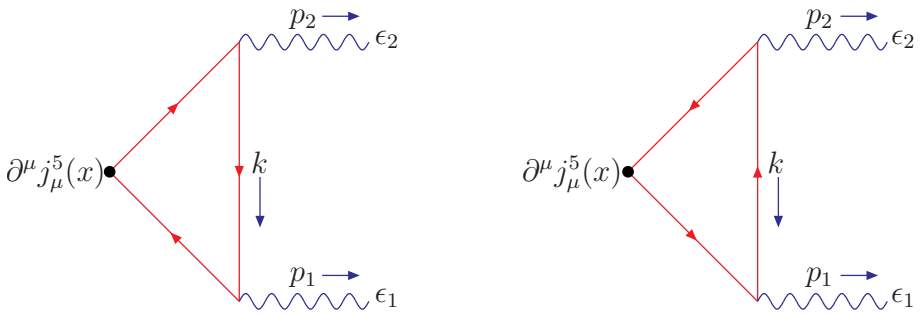

Figure 10: Feynman diagrams for the matrix element $\langle p_1, \epsilon_1, a; p_2 \epsilon_2, b | \partial^\mu j^5_\mu | 0 \rangle$

These diagrams give

$$\partial^\mu \langle p_1, \epsilon_1, a; p_2, \epsilon_2, b | j^5_\mu(x) | 0 \rangle \;=\; -e^{-i(p_1+p_2)\cdot x}\,\mathrm{Tr}(\tau^a \tau^b) \int \frac{d^d k}{(2\pi)^d} \frac{\mathcal{N}}{k^2 (k+p_2)^2 (k-p_1)^2}, \quad (10.25)$$

where d is the number of dimensions, and the numerator $\mathcal{N}$ is

$$\begin{aligned} \mathcal{N} &= g^2 \mathrm{Tr}\left[\not{k} (\not{p}_1 + \not{p}_2)\, \gamma^5\, (\not{k} + \not{p}_2)\, \not{\epsilon}_2\, (\not{k} - \not{p}_1)\, \not{\epsilon}_1 \right] + (p_1 \leftrightarrow -p_2,\ \epsilon_1 \leftrightarrow \epsilon_2) \\ &= 8 g^2 i \epsilon_{\mu\nu\rho\sigma} \left[p_1^\mu p_2^\nu k^\rho k^\lambda \left(\epsilon_1^\lambda \epsilon_2^\sigma - \epsilon_2^\lambda \epsilon_1^\sigma \right) - 2 p_1^\mu p_2^\nu \epsilon_1^\rho \epsilon_2^\sigma k^2 - k^2 \left(p_1^\mu + p_2^\mu \right) \epsilon_1^\rho \epsilon_2^\sigma \right]. \quad (10.26) \end{aligned}$$

In obtaining this numerator, we have used the on-shell conditions for the (massless) external gauge particles,

$$p_1 \cdot \epsilon_1 \;=\; p_2 \cdot \epsilon_2 \;=\; 0, \quad p_1^2 \;=\; p_2^2 \;=\; 0$$

We have the following relations between the integrals over the loop momentum k:

$$\int \frac{d^d k}{(2\pi)^d} \frac{k^\mu}{(k-p_1)^2 (k+p_2)^2} \;=\; \frac{(p_1^\mu - p_2^\mu)}{2} \int \frac{d^d k}{(2\pi)^d} \frac{1}{(k-p_1)^2 (k+p_2)^2} \quad (10.27)$$

and

$$d\, \epsilon_{\mu\nu\rho\sigma} \int \frac{d^d k}{(2\pi)^d} \frac{p_1^\mu p_2^\nu k^\rho k^\lambda}{k^2 (k-p_1^2)(k+p_2)^2} \;=\; \epsilon_{\mu\nu\lambda\sigma} \int \frac{d^d k}{(2\pi)^d} \frac{p_1^\mu p_2^\nu k^2 - (p_1^\mu + p_2^\nu) k^\nu}{k^2 (k-p_1^2)(k+p_2)^2} \quad (10.28)$$

Piecing together, we have

$$\begin{aligned} \partial^\mu \langle p_1, \epsilon_1, a; p_2, \epsilon_2, b | j^5_\mu(x) | 0 \rangle \;&=\; -ig^2 \frac{1}{2} \delta_{ab} e^{-i(p_1+p_2)\cdot x} \epsilon_{\mu\nu\rho\sigma} p_1^\mu p_2 \nu \epsilon_1^\rho \epsilon_2^\sigma \left(\frac{16}{d} - 4 \right) \\ &\quad \times \int \frac{d^d k}{(2\pi)^d} \frac{1}{(k-p_1)^2 (k+p_2)^2} \quad (10.29) \end{aligned}$$

Note that if we set $d = 4$ this matrix element vanishes. However the integral has a UV divergence, which manifests itself as a pole at $d = 4$

$$\int \frac{d^d k}{(2\pi)^d} \frac{1}{(k-p_1)^2 (k+p_2)^2} \;=\; \frac{-i}{16\pi^2} \frac{2}{(d-4)} + \cdots$$

so that we are left with

$$\partial^\mu \langle p_1, \epsilon_1, a; p_2, \epsilon_2, b | j^5_\mu(x) | 0 \rangle \;=\; \frac{g^2}{8\pi^2} \delta_{ab} e^{-i(p_1+p_2)\cdot x} \epsilon_{\mu\nu\rho\sigma} p_1^\mu p_2^\nu \epsilon_1^\rho \epsilon_2^\sigma \tag{10.30}$$

Consider now the matrix element

$$\langle p_1, \epsilon_1, a; p_2, \epsilon_2, b | \mathrm{Tr} \left\{ \mathbf{F}^{\mu\nu} \tilde{\mathbf{F}}_{\mu\nu} \right\} | 0 \rangle$$

Expanding the quantum field $\hat{\mathbf{A}}_\mu$ in terms of creation and annihilation operators, we can show that

$$\langle p_1, \epsilon_1, a; p_2, \epsilon_2, b | \mathrm{Tr} \left\{ \mathbf{F}^{\mu\nu} \tilde{\mathbf{F}}_{\mu\nu} \right\} | 0 \rangle \;=\; \delta_{ab} e^{-i(p_1+p_2)\cdot x} \epsilon_{\mu\nu\rho\sigma} p_1^\mu p_2^\nu \epsilon_1^\rho \epsilon_2^\sigma \tag{10.31}$$

Comparing (10.30) and (10.31) we can make the identification

$$\partial \cdot j^5 \;=\; \frac{g^2}{8\pi^2} \mathrm{Tr}\{ \mathbf{F}^{\mu\nu} \tilde{\mathbf{F}}_{\mu\nu} \} \tag{10.32}$$

Since $\mathbf{F}_{\mu\nu}$ and $\tilde{\mathbf{F}}_{\mu\nu}$ each contain a term which is quadratic in the gauge-field, there will also be non-zero matrix elements of the operator $\partial^\mu j^5_\mu$ between the vacuum and states containing three and possibly four external gauge-bosons. However, it has been shown that there are '*no* corrections to the anomaly found here from higher order (multi-loop) Feynman diagrams.

So far, we have only considered one multiplet of massless fermions. If we have N_f such multiplets (N_f flavours in QCD), then the divergence of the axial current acquires a factor of N_f and (10.32) generalises to

$$\partial \cdot j^5 \;=\; \frac{g^2 N_f}{8\pi^2} \mathrm{Tr}\{ \mathbf{F}^{\mu\nu} \tilde{\mathbf{F}}_{\mu\nu} \} \tag{10.33}$$

It is worth noting that although the axial current is not conserved, we can construct a conserved current

$$\tilde{j}^5_\mu \;\equiv\; j^5_\mu - 2N_f K_\mu \tag{10.34}$$

where K_μ is defined in (10.7) and its divergence is given in (10.9). However, whereas this current is indeed conserved, it is *not* gauge invariant as can be seen explicitly by performing a gauge transformation a gauge transformation on the vector K_μ). So we see that the existence of this anomaly means that we can *either* maintain gauge invariance in higher orders *or* maintain (a modified) axial $U(1)$ invariance but not both.

10.3.1 The U(1) Problem

If we have N (almost) massless fermions, Ψ^a then there is an (approximate) global $U(N)_L \times U(N)_R$ invariance since here is an invariance under a transformation which rotates either the left-handed or right-handed fermions into each other.

This symmetry is broken spontaneously by the presence of a condensate $\langle 0|\overline{\Psi}_a\Psi^a|0\rangle$. which brakes the axial $U(N)$. By Goldstone's theorem, this should generate N^2 (almost) massless pseudoscalar bosons. For $N = 3$ we can identify 8 of these as the pseudoscalar octet – $\pi^{\pm}$, π^0, $K^{\pm}$, K^0, $\overline{K^0}$, η. The expected ninth Goldstone boson is absent (the mass of the η' is too large to be identified as a Goldstone boson.)

However, we see from (10.33) that axial $U(1)$ is broken by the anomaly. On the other hand we see from (10.34) that there is a current which is not anomalous but is gauge dependent. The spontaneous breaking of the modified $U(1)$ for which $\tilde{j}^5_\mu$ is the Noether current *does* generate a Goldstone boson, but not a Goldstone boson that appears in physical - i.e. gauge invariant - states. The divergence of the modified axial current caused by an axial $U(1)$ transformation can be undone by a shift in θ in the θ-vacuum. In some sense, fixing θ is the global equivalent of making a gauge choice, and the excitations of the unphysical axial $U(1)$ Goldstone boson correspond to oscillations in θ. In this sense , instantons provide a solution to the $U(1)$ problem.

10.4 Instantons with Chiral Fermions

10.4.1 Fermionic zero modes

If we add a fermion Ψ to the pure gauge theory, the generating functional is given by (10.22). The path integral over the fermion field has a pre-factor (in the numerator for fermions, which are treated using Grassman variables, is

$$\det \not{\mathbf{D}} \;=\; \prod_i \lambda_i,$$

where λ_i are the eigenvalues of $\not{\mathbf{D}}$.

For an instanton background gauge-field with centre x_0 and size ρ, the operator $i\not{\mathbf{D}} = i\mathbb{1}\not{\partial} - g\not{\mathbf{A}}_I$ has is an eigenfunction with eigenvalue zero (a zero mode). This zero mode (which depends on the centre x_0 and size ρ, of the instanton,has right-handed chirality, and may be written (in the Weyl representation representation)

$$\Psi_0^{(\pm)}(x, x_0, \rho) \;=\; \begin{pmatrix} \chi_0^{(\pm)}(x, x_0, \rho) \\ 0 \end{pmatrix} \tag{10.35}$$

where the index $(\pm)$ refers to the third component of the $SU(2)$ subgroup of the gauge group.

Whereas it is not possible to have purely right-handed eigenfunctions, Ψ_i, of $\not{\mathbf{D}}$ with non-zero eigenvalue, λ_i because

$$\not{\mathbf{D}}\gamma^5\Psi_i \;=\; -\lambda_i\gamma^5\Psi_i,$$

so that Ψ_i, $(i \neq 0)$ cannot be an eigenstate of $(1 \pm \gamma^5)$. But if $\lambda_i = 0$ then we can have eigenfunctions which are also eigenfunctions of γ_5 with eigenvalue +1 for right-handed spinors and -1 for left-handed spinors.

In the singular gauge where $A^a_{I\mu}$ is given by (10.14), the normalised spinor, $\chi_0^{(i)}(x,\rho)$ is given by

$$\chi_0^{(\pm)}(x,x_0,\rho) \;=\; \frac{1}{\sqrt{2\pi^2}}\frac{\rho}{\left((x-x_0)^2+\rho^2\right)^{3/2}}(x-x_0)\cdot\sigma\left(\sigma^2\chi^{(\pm)}\right), \tag{10.36}$$

where $\sigma_\mu \equiv (\mathbb{1}, -i\boldsymbol{\sigma})$ and $\chi^{(\pm)}$ is the $SU(2)$ spinor of the fermion (assumed to be in the defining representation of $SU(2)$). Explicitly

$$\begin{aligned}\sigma^2\chi^+ &= \begin{pmatrix} 0 \\ i \end{pmatrix} \\ \sigma^2\chi^- &= \begin{pmatrix} -i \\ 0 \end{pmatrix}.\end{aligned} \tag{10.37}$$

The spinor χ_0 is normalised such that

$$\int d^4x \chi_0^{a\dagger}(x,x_0,\rho)\chi_0^b(x,x_0,\rho) \;=\; \delta^{ab} \tag{10.38}$$

In an anti-insanton background the fermionic zero mode is left-handed.

This is an example of the Atiyah-Singer index theorem which tells us that for any gauge-field configuration with N_f multiplets of massless fermions, for which

$$\frac{g^2}{16\pi^2}\int d^4x \mathrm{Tr}\{\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\} \;=\; \Delta n$$

the number of left-handed fermionic zero modes, n_L and the number of right-handed fermionic zero modes, n_R, are related by

$$n_R - n_L \;=\; \Delta n \tag{10.39}$$

10.4.2 Axial Charge Violation

The existence of this zero mode means that in the absence of a source for the fermion fields that instanton transition between vacua in adjacent homotopy classes vanishes. This is because the fermionic contibution to the generating functional

$$\int \mathcal{D}[\overline{\Psi}]\mathcal{D}[\Psi]\exp\left\{-\int d^4x \overline{\Psi}(x) i \not{D}\Psi(x)\right\} \;=\; \int d\overline{c}_0 dc_0 \prod_{i=1}^{\infty} d\overline{c}_i dc_i \exp\left\{-\overline{c}_i\lambda_i c_i\right\} \tag{10.40}$$

and the integral over the Grassman variables $\overline{c_0}, c_0$ vanishes.

We can, however, obtain non-zero vacuum expectation values of an operator which is bilinear in the fermion field and which is not invariant under axial $U(1)$ transformations (i.e. it violates the conservation of axial charge), in the presence of an instanton.

Consider the matrix element

$$\langle (n+1), \tau\to\infty \left|\mathcal{O}_{(\Delta Q^5=2)}\right| n, \tau\to-\infty\rangle$$

where the axial-charge violating operator $\mathcal{O}_{(\Delta Q^5=2)}$,given by

$$\mathcal{O}_{(\Delta Q^5=2)} \;=\; \overline{\Psi}(x)\gamma^0\frac{(1+\gamma^5)}{2}\Psi(x), \tag{10.41}$$

converts a left-handed fermion into a right-handed fermion.

The fermionic part of the path integral is

$$\int \mathcal{D}[\overline{\Psi}]\mathcal{D}[\Psi]\,\overline{\Psi}(x_1)\gamma^0\frac{(1+\gamma^5)}{2}\Psi(x_1)\exp\left\{-\int d^4x\overline{\Psi}(x)i\not{D}\Psi(x)\right\}$$

Now when we expand the fermion fields in terms of eigenstates of $i\not{D}$, we get a term in the integrand proportional to the coefficients, c_0 and $\overline{c}_0$ of the fermionic zero mode so that we now have (for an instanton of size ρ centred at x_0),

$$\begin{aligned}\int\prod_i d\overline{c}_i dc_i\,\overline{c}_0 c_0\chi^\dagger(x_1,x_0,\rho)\chi(x_1,x_0,\rho)\exp\{-\overline{c}_i\lambda_i c_i\} \;&=\\ \det(i\not{D}')\chi^\dagger(x_1,x_0,\rho)\chi(x_1,x_0,\rho),&\end{aligned} \tag{10.42}$$

where the $\not{D}'$ indicates the operator with the zero mode removed, and χ_0 is the spinor for the (right–handed) fermion zero mode given by (10.36).

To calculate the value of the matrix element of this operator, we multiply by the transition amplitude due to an instanton centred at x_0 of size ρ and integrate over the collective coordinates, x_0 and ρ to obtain

$$\begin{aligned}&\langle(n+1),\tau\to\infty|\overline{\Psi}(x_1)\gamma^0\frac{(1+\gamma^5)}{2}\Psi(x_1)|n,\tau\to-\infty\rangle \;=\\ K\int d^4x_0\int\frac{d\rho}{\rho^5}\rho\left(\frac{\det(i\not{D}')}{\rho\det(i\not{\partial})}\right)\chi_0^\dagger(x_1,x_0,\rho)\chi_0(x_1,x_0,\rho)\left(\frac{8\pi^2}{g^2(1/\rho)}\right)^4\exp\left\{-\frac{8\pi^2}{g^2(1/\rho)}\right\}&\\ =\; K\int\frac{d\rho}{\rho^5}\rho\left(\frac{\det(i\not{D}')}{\rho\det(i\not{\partial})}\right)\left(\frac{8\pi^2}{g^2(1/\rho)}\right)^4\exp\left\{-\frac{8\pi^2}{g^2(1/\rho)}\right\}&\end{aligned} \tag{10.43}$$

where in the last step we have used the normalisation property, (10.38), of the zero-mode spinor to perform the integral over the instanton centre.

We have divided by the determinant of the Dirac operator $\not{\partial}$ in the absence of a background instanton field and explicitly pulled out a factor of ρ to indicate that the dimension of det $\not{\partial}$ is one greater than the dimension of det $\not{D}'$ since it has one more non-zero eigenvalue so that for an instanton of size ρ we expect

$$\det(i\not{\partial}) \;\sim\; \rho\det(i\not{D}').$$

This vacuum expectation value is the amplitude for a right-handed fermions at x_2 to propagate into a left-handed fermion at x_1. By crossing symmetry this may also be used to calculate a non-zero transition amplitude from an initial state with a given number of

fermions and anti-fermions to a final state with an additional left-handed fermion and left-handed anti-fermion - again changing the axial charge by two units.

In the case of an anti-instanton we get the Hermitian conjugate of (10.43) where we get a non-zero matrix element for the operator

$$\mathcal{O}_{(\Delta Q^5=-2)} \;=\; \overline{\Psi}(x)\gamma^0\frac{(1-\gamma^5)}{2}\Psi(x), \tag{10.44}$$

between vacuum states $\langle(n-1)|$ and $|n>$

As in the case of the periodic potential we can sum over all sequences of instantons and anti-instantons and construct the vacuum expectation value for the θ-vacua. This generates an extra effective term in the effective action

$$\begin{aligned}\Delta\mathcal{L}_I^f \;\equiv\; & K\int\frac{d\rho}{\rho^5}\rho\left(\frac{\det(i\not{D}')}{\rho\det(i\not{\partial})}\right)\left(\frac{8\pi^2}{g^2(1/\rho)}\right)^4\exp\left\{-\frac{8\pi^2}{g^2(1/\rho)}\right\}\\ & \times\left(\overline{\Psi}(x)\gamma^0\Psi(x)\cos\theta+i\overline{\Psi}(x)\gamma^0\gamma^5\Psi(x)\sin\theta\right)\end{aligned} \tag{10.45}$$

10.4.3 Several flavours

If we have two multiplets of massless fermions, Ψ^1, Ψ^2, then we can only have a non-zero matrix element if we have one power of each of $\overline{\Psi}^1$, Ψ^1, $\overline{\Psi}^2$, Ψ^2, in the fermion path integral in order for the path integral to yield a non-zero result when integrated over the Grassman coefficients of the zero modes for both the fermions. In that case we obtain a non-zero vacuum expectation value of the form

$$\langle 0|\overline{\Psi}^1(x_1)\gamma^0\frac{(1+\gamma^5)}{2}\Psi^1(x_1)\overline{\Psi^2}(x_2)\gamma^0\frac{(1+\gamma^5)}{2}\Psi^2(x_2)|0\rangle$$

We could also have the same non-zero vacuum expectation value of the term

$$-\langle 0|\overline{\Psi}^1(x_1)\gamma^0\frac{(1+\gamma^5)}{2}\Psi^2(x_1)\overline{\Psi}^2(x_2)\gamma^0\frac{(1+\gamma^5)}{2}\Psi^1(x_2)|0\rangle,$$

where the minus sign in from arises because it has been necessary to interchange the order of two of the Grassman source functions to obtain that operator. This operator carries axial charge 4.

In general, if we have N_f fermion flavours, Ψ^l, $l=1\cdots N_f$ then the operator which has a non-zero vacuum expectation value is

$$\det_{kl}\overline{\Psi}^k\gamma^0\frac{(1+\gamma^5)}{2}\Psi^l,$$

which carries an axial charge of $2N_f$ This is expected from the anomaly of the axial current. Taking the divergence of both sides of (10.34) we have

$$0 \;=\; \partial\cdot j^5(x) \;-\; 2N_f\partial\cdot K(x)$$

and integrating over all space-time, using Gauss theorem we have

$$\Delta Q^5 \equiv Q^5(t\to\infty) - Q^5(t\to-\infty) = 2N_f\left(K_0(t\to\infty) - K_0(t\to-\infty)\right) = 2N_f, \quad (10.46)$$

for a single instanton transition.

10.4.4 Baryogenesis

This also has consequences for baryogenesis, when applied to the Standard Model of electroweak interactions, in which the weak $SU(2)$ gauge field couples to left-handed fermions only. In such a case, we see from the triangle calculation of the previous section that we can also have an anomaly in a vector fermion current

$$j_\mu = \overline{\Psi}\gamma_\mu\Psi$$

The anomaly in this current from the interaction of the left-handed fermions with the weak $SU(2)$ gauge fields is given by

$$\partial\cdot j = N_f\frac{g_W^2}{8\pi^2}\frac{1}{2}\mathrm{Tr}\left(\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}\right) \quad (10.47)$$

where the field strength $\mathbf{F}^{\mu\nu}$ now refers to the weak $W's$, N_f is the number of weak isodoublets. The factor of $\frac{1}{2}$ appears because only the left-handed fermions interact with the weak gauge fields. An instanton can generate a transition amplitude which violates fermion number by N_f, but electric charge and the third component of weak isospin must clearly be conserved.

For a one-generation model with three doublets of quarks and one doublet of leptons an operator such as $u^r u^y d^b e$ or $u^r d^y d^b \nu$ can have a non-zero vacuum expectation value and this facilitates a process such as a positron converting into a proton (consisting of 2 u-quarks and a d-quark). If we have two generations of (almost) massless quarks a typical reaction could be

$$e^+ + \overline{\nu}_\mu = u^r + u^y + d^b + \tilde{s}^r + \tilde{s}^y + \tilde{s}^b$$

where $\tilde{s}$ is the Cabbibo superposition

$$\tilde{s} = s\cos\theta_C - d\sin\theta_C$$

so that there is a smaller (suppressed by three powers of $\sin\theta_C$) amplitude for the annihilation of a positron and (muon-type) into a proton and a neutron.

Note that in any case, the instanton amplitude in weak interactions is extremely small due to the instanton action factor

$$\exp\left\{-\frac{8\pi^2}{g_W^2}\right\} \approx 10^{-86}$$

10.4.5 Light quarks

The masses of fermion fields are never exactly zero. If we have a small mass m for the fermions then the "zero"-mode no longer has eigenvalue zero but the smallest eigenvalue is m. In this case we *can* have instanton transitions without introducing an operator that violates axial charge. The generating functional is proportional to m and by dimensional arguments for an instanton of size ρ, Green's functions constructed from this generating functional are suppressed by a factor of $m\rho$. Since we expect the instanon size to be cut off at $\rho \sim 1/\Lambda_{\rm QCD}$ we can use the massless quark approximation provided the fermion mass, m is much less than $\Lambda_{\rm QCD}$.

10.5 The strong CP problem: Peccei-Quinn Theory

The small amount of CP violation observed in weak interactions is encoded in the standard model by allowing some of the elements of the fermion mass matrix to be complex.

However, we are at liberty to add to the Lagrangian density the gauge invariant term

$$\Delta\mathcal{L}(\theta) \;\equiv\; \frac{g^2}{16\pi^2}\theta\,{\rm Tr}(\mathbf{F}^{\mu\nu}\tilde{\mathbf{F}}_{\mu\nu}) \tag{10.48}$$

This is a total derivative so that its contribution to the action is always the Pontryagin index, Δn, of the instanton. The matrix element of such a term between θ- vacua with $\theta = \theta'$ is then proportional to

$$\sum_{n_1}\sum_{n_2}\exp\left\{in_1\theta'\right\}\exp\left\{-in_2\theta'\right\}\exp\left\{i\left(n_2-n_1\right)\theta\right\} \;=\; \delta(\theta-\theta') \tag{10.49}$$

which tells us that for a given θ-vacuum the value of θ in the new term must be equal to the vacuum θ value.

However, the addition of the term $\Delta\mathcal{L}(\theta)$ violates CP conservation and since θ can take any value between 0 and 2π, this CP violation can be large in conflict with experimental observation, which shows that CP violating amplitudes are extremely weak.. This is called the "strong CP problem".

The most popular solutions to this problem are variations of the Peccei-Quinn model. In this model a second Higgs doublet, Φ_2 is added to the SM Higgs doublet Φ_1. This introduces a $U(1)$ transformation, $U(1)_{PQ}$ which changes the relative phase of the two scalar multiplets.

The scalar potential $V(\Phi_1,\Phi_2)$ is invariant under two $U(1)$ transformations corresponding to a change of phase in both of the scalar doublets'

$$\Phi_1 \;\to\; e^{-i\alpha_1}\Phi_1, \quad \Phi_2 \;\to\; e^{-i\alpha_2}\Phi_2$$

The minimum of the potential for which

$$|\langle\Phi_1\rangle| \;=\; v\cos\beta, \qquad |\langle\Phi_2\rangle| \;=\; v\sin\beta,$$

($v = 2M_W/g_W$) breaks the symmetry from $SU(2) \times U(1) \times U(1)_{PQ}$ g to the electromagnet gauge symmetry $U(1)_{em}$. This breaking generates two massless neutral Goldstone bosons, a_1, a_2. The linear combination

$$a_z \;\equiv\; a_1 \cos\beta - a_2 \sin\beta,$$

is absorbed by the Z-boson, which acquires a mass. The other orthogonal linear combination

$$a \;\equiv a_1 \sin\beta + a_2 \cos\beta$$

remains massless, but is a physical particle known as the "axion".

Only the right-handed fermions transform under a $U(1)_{PQ}$ transformation with parameter α:

$$u_R \;\to\; e^{i\alpha\tan\beta} u_R, \quad d_R \;\to\; e^{i\alpha\cot\beta} d_R, \quad e_R \;\to\; e^{i\alpha\cot\beta} e_R \tag{10.50}$$

and the axion transforms as

$$a \;\to\; a - v\alpha \tag{10.51}$$

The $U(1)_{PQ}$ current

$$j^{PQ}_\mu \;=\; \tan\beta\, \overline{u}^i \gamma_\mu \frac{(1+\gamma^5)}{2} u_i + \cot\beta\, \overline{d}^i \gamma_\mu \frac{(1+\gamma^5)}{2} d_i + \cot\beta\, \overline{e}\gamma_\mu \frac{(1+\gamma^5)}{2} e - v\,\partial_\mu a, \quad (i = 1\cdots 3) \tag{10.52}$$

This current is anomalous and its divergence couples both to gluons and photons via triangle diagrams.

For one generation we find

$$\partial \cdot j^{PQ} \;= \frac{g^2}{8\pi^2 \sin(2\beta)} \mathrm{Tr}\left\{ \mathbf{F}^{\mu\nu} \tilde{\mathbf{F}}_{\mu\nu} \right\} + \frac{e^2}{6\pi^2 \sin(2\beta)} F^{\mu\nu}_\gamma \tilde{F}_{\gamma\mu\nu} \tag{10.53}$$

(N.B. $\tan\beta + \cot\beta = 2/\sin(2\beta)$).

We compensate for this anomaly by adding to the QCD Lagrangian density (omitting the electromagnetic anomaly) the effective term

$$\Delta\mathcal{L}_{PQ} \;=\; \frac{a}{v} \frac{g^2}{8\pi^2 \sin(2\beta)} \mathrm{Tr}\left(\mathbf{F}^{\mu\nu} \tilde{\mathbf{F}}_{\mu\nu} \right) \tag{10.54}$$

The change in $\Delta\mathcal{L}_{PQ}$ under a $U(1)^{PQ}$ is then equal and opposite to $\partial \cdot j^{PQ}$

With this term added to the effective action, the effect of sequences of instantons and anti-instantons changes from

$$\Delta\mathcal{L}(\theta) \;\propto \cos\theta,$$

(see (10.21)) to

$$\Delta\mathcal{L}(\theta) \;\propto \cos\left(\theta + \frac{2}{v \sin(2\beta)} a \right) \tag{10.55}$$

This effective potential leads to a vacuum expectation value for the axion field, a, corresponding to a turning point of $\Delta\mathcal{L}(\theta)$ at

$$\langle a \rangle \;=\; -\frac{\sin(2\beta)}{2} v\theta \tag{10.56}$$

For this value of the axion field, the two terms in the effective Lagrangian density which violate CP conservation, $\Delta\mathcal{L}(\theta)$ and $\Delta\mathcal{L}^{PQ}$ cancel out and there is *no* QCD contribution to CP violation.

The matrix element of the Peccei-Quinn current between the vacuum and a single axion with momentum p is

$$\langle 0 \left| j_\mu^{PQ}(0) \right| a(p) \rangle \;=\; v p_\mu \tag{10.57}$$

comparing this with the matrix element of the axial current between the vacuum and a single pion state

$$\langle 0 \left| j_\mu^{5}(0) \right| \pi(p) \rangle \;=\; f_\pi p_\mu,$$

where f_π is the pion decay constant, we see that we can interpret the vacuum expectation value of the SM, v (~ 246 GeV) as the decay constant of the axion. The pion is not strictly massless because the light quarks have a small mass m_u, m_d. Chiral perturbation theory gives the pion mass, m_π as

$$m_\pi^2 \;=\; \frac{\langle 0 \left| \overline{u}u + \overline{d}d \right| 0 \rangle}{f_\pi^2} (m_u + m_d) \tag{10.58}$$

This leads to an expression for the axion mass, m_a

$$m_a \;=\; \frac{f_\pi}{v} m_\pi \tag{10.59}$$

A more careful calculation introduces a factor of 0.5 and the axion mass is estimated to be about 25 keV. Such an axion would have already been observed, for ecample in the decay

$$K^+ \;\rightarrow\; \pi^+ + a.$$

The absence of such events implies that this simple model does not work but several alternative models in which the axion is "invisible" have replaced it - but all of these are based of the principle of a spontaneously broken Peccei-Quinn $U(1)$ symmetry.