5 Path Integrals in Quantum Mechanics and Quantum Field Theory

In the past chapter we gave a summary of the Hilbert space picture of Quantum Mechanics and of a Scalar Quantum Field Theory. Here we will present the *Path Integral* picture of Quantum Mechanics ans Scalar Quantum Field Theory.

The Path Integral picture is important for two reasons. First, it offers an alternative, complementary, picture of Quantum Mechanics in which the role of the classical limit is apparent. Secondly, it gives a direct route to the study regimes where perturbation theory is either inadequate or fails completely. A standard approach to these problems is the WKB approximation (Wentzel, Kramers and Brillouin). As it happens, it is extremely difficult (if not impossible) the generalize the WKB approximation to a Quantum Field Theory. Instead, the non-perturbative treatment of the Feynman path integral, which is equivalent to WKB, is generalizable to non-perturbative problems in QFT. In this chapter we will use path integrals only for bosonic systems, such as scalar and abelian gauge fields. In the following chapters we will also give a full treatment of the path integral, including its applications to fermionic fields, non-relativistic many body systems, and Abelian gauge fields. Non-Abelian gauge fields will be discussed in the following course, Physics 583.

5.1 Path Integrals and Quantum Mechanics

Consider a simple quantum mechanical system whose dynamics can be described by a (generalized) time-dependent coordinate operator $\hat{q}(t)$, *i.e.,* the position operator in the Heisenberg representation. We will denote by $|q,t\rangle$ an eigenstate of $\hat{q}(t)$ with eigenvalue q,

$$\hat{q}(t)|q,t\rangle = q|q,t\rangle \tag{1}$$

We want to compute the amplitude

$$F(q_f,t_f|q_i,t_i) = \langle q_f,t_f|q_i,t_i\rangle \tag{2}$$

Let $\hat{q}_S$ be the Schrödinger operator, related to the Heisenberg operator $\hat{q}(t)$ by the action of the time evolution operator:

$$\hat{q}(t) = e^{i\hat{H}t/\hbar}\hat{q}_S\, e^{-i\hat{H}t/\hbar} \tag{3}$$

and whose eigenstates are $|q\rangle$,

$$\hat{q}_S|q\rangle = q|q\rangle \tag{4}$$

The states $|q\rangle$ and $|q,t\rangle$ are related *via* the evolution operator

$$|q\rangle = e^{-i\hat{H}t/\hbar}|q,t\rangle \tag{5}$$

Therefore the amplitude $F(q_f,t_f|q_i,t_i)$ is a matrix element of the evolution operator

$$F(q_f,t_f|q_i,t_i) = \langle q_f|e^{i\hat{H}(t_i-t_f)/\hbar}|q_i\rangle \tag{6}$$

The amplitude $F(q_f, t_f|q_i, t_i)$ has a simple physical interpretation. Let us set, for simplicity, $|q_i, t_i\rangle = |0, 0\rangle$ and $|q_f, t_f\rangle = |q, t\rangle$. Then, from the definition of this matrix element, we find out that it obeys

$$\lim_{t\to 0} F(q, t|0, 0) = \langle q|0\rangle = \delta(q) \tag{7}$$

Furthermore, after some algebra we also find that

$$\begin{aligned} i\hbar\frac{\partial F}{\partial t} &= i\hbar\frac{\partial}{\partial t}\langle q, t|0, 0\rangle \\ &= i\hbar\frac{\partial}{\partial t}\langle q|e^{-i\hat{H}t/\hbar}|0\rangle \\ &= \langle q|\hat{H}e^{-i\hat{H}t/\hbar}|0\rangle \\ &= \int dq'\langle q|\hat{H}|q'\rangle\langle q'|e^{-i\hat{H}t/\hbar}|0\rangle \end{aligned} \tag{8}$$

where we have used that, since $\{|q\rangle\}$ is a complete set of states, the identity operator I has the expansion, called the *resolution of the identity*,

$$I = \int dq'|q'\rangle\langle q'| \tag{9}$$

Here we have assumed that the states are orthonormal, *i.e.,*

$$\langle q|q'\rangle = \delta(q - q') \tag{10}$$

Hence,

$$i\hbar\frac{\partial F}{\partial t} = \int dq'\langle q|\hat{H}|q'\rangle F(q', t|0, 0) \equiv \hat{H}_q F(q, t|0, 0) \tag{11}$$

In other terms, $F(q, t|0, 0)$ is the solution of the Schrödinger Equation that satisfies the initial condition of Eq. 7. The amplitude $F(q, t|0, 0)$ is called the *Schrödinger Propagator*. Let us next define a *partition* of the time interval $[t_i, t_f]$ into N intervals of length Δt,

$$t_f - t_i = N\Delta t \tag{12}$$

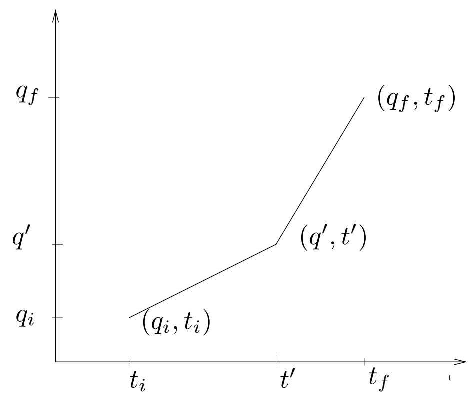
Let $\{t_j\}$ (with $j = 0, \ldots, N + 1$) denote a set of points in the interval $[t, t_f]$, such that

$$t_i = t_0 \leq t_1 \leq \ldots \leq t_N \leq t_{N+1} = t_f \tag{13}$$

Clearly, $t_k = t_0 + k\Delta t$ (for $k = 1, \ldots, N + 1$.

The superposition principle tells us that

$$F(q_f, t_f|q_i, t_i) = \int dq'\langle q_f, t_f|q', t'\rangle\langle q', t'|q_i, t_i\rangle \tag{14}$$



where we have inserted I in the form of the resolution of the identity of Eq. 14. By repeating this process many times we find

$$
\begin{aligned}
F(q_f, t_f|q_i, t_i) = \int dq_1 \dots dq_N \qquad & \langle q_f, t_f|q_N, t_N\rangle\langle q_N, t_N|q_{N-1}, t_{N-1}\rangle \times \dots \\
& \times \dots \langle q_j, t_j|q_{j-1}, t_{j-1}\rangle \dots \langle q_1, t_1|q_i, t_i\rangle
\end{aligned}
\tag{15}
$$

Each factor $\langle q_j, t_j|q_{j-1}, t_{j-1}\rangle$ has the form

$$
\langle q_j, t_j|q_{j-1}, t_{j-1}\rangle = \langle q_j|e^{-i\hat{H}(t_j-t_{j-1})/\hbar}|q_{j-1}\rangle \equiv \langle q_j|e^{-i\hat{H}\Delta t/\hbar}|q_{j-1}\rangle \tag{16}
$$

In the limit $N \to \infty$, with $|t_f - t_i|$ fixed and finite, the interval Δt becomes infinitesimally small and $\Delta t \to 0$. Hence, as $N \to \infty$ we can write the approximate expression for $\langle q_j, t_j|q_{j-1}, t_{j-1}\rangle$,

$$
\begin{aligned}
\langle q_j, t_j|q_{j-1}, t_{j-1}\rangle &= \langle q_j|e^{-iH\Delta t/\hbar}|q_{j-1}\rangle \\
&= \langle q_j|I - i\frac{\Delta t}{\hbar}\hat{H} + O((\Delta t)^2)|q_{j-1}\rangle \\
&= \delta(q_j - q_{j-1}) - i\frac{\Delta t}{\hbar}\langle q_j|\hat{H}|q_{j-1}\rangle + O((\Delta t)^2)
\end{aligned}
\tag{17}
$$

which becomes asymptotically exact as $N \to \infty$.

We can also introduce a complete set of momentum eigenstates $\{|p\rangle\}$ and their resolution of the identity

$$
I = \int_{-\infty}^{\infty} dp \; |p\rangle\langle p| \tag{18}
$$

Recall that the overlap between $|q\rangle$ and $|p\rangle$ is

$$
\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \; e^{ipq/\hbar} \tag{19}
$$

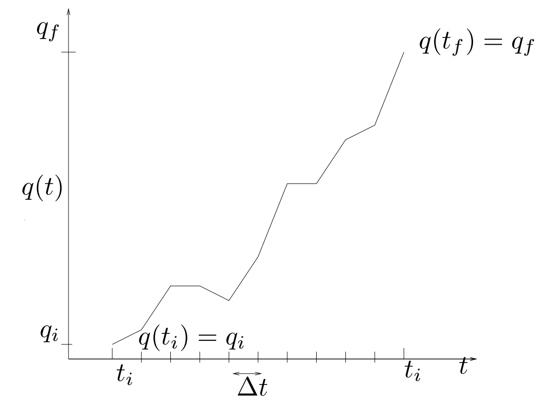


Figure 1: A history $q(t)$ of the system.

For a typical Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \tag{20}$$

its matrix elements are

$$\langle q_j|\hat{H}|q_{j-1}\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\; e^{ip(q_j - q_{j-1})/\hbar}\; \left[\frac{p^2}{2m} + V(q_j)\right] \tag{21}$$

Within the same level of approximation we can also write

$$\langle q_j, t_j|q_{j-1}, t_{j-1}\rangle \approx \int \frac{dp}{2\pi\hbar} \exp\left[i\left(\frac{p}{\hbar}(q_j - q_{j-1}) - \Delta t\; H\left(p, \frac{q_j + q_{j-1}}{2}\right)\right)\right] \tag{22}$$

where we have introduce the "mid-point rule" which amounts to the replacement $q_j \to \frac{1}{2}(q_j + q_{j-1})$ inside the Hamiltonian $H(p, q)$. Putting everything together we find that the matrix element $\langle q_f, t_f|q_i, t_i\rangle$ becomes

$$\begin{aligned}\langle q_f, t_f|q_i, t_i\rangle \;\; &= \;\; \lim_{N\to\infty} \int \prod_{j=1}^{N} dq_j \int_{-\infty}^{\infty} \prod_{j=1}^{N+1} \frac{dp_j}{2\pi\hbar} \\ &\qquad \exp\left\{\frac{i}{\hbar} \sum_{j=1}^{N+1} \left[p_j(q_j - q_{j-1}) - \Delta t\; H\left(p_j, \frac{q_j + q_{j-1}}{2}\right)\right]\right\}\end{aligned} \tag{23}$$

Therefore, in the limit $N \to \infty$, holding $|t - t_f|$ fixed, the amplitude $\langle q_f, t_f|q_i, t_i\rangle$ is given by the (formal) expression

$$\langle q_f, t_f|q_i, t_i\rangle = \int \mathcal{D}p\mathcal{D}q\;\; e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\,[p\dot{q} - H(p, q)]} \tag{24}$$

where we have used the notation

$$\mathcal{D}p\mathcal{D}q \equiv \lim_{N\to\infty} \prod_{j=1}^{N} \frac{dp_j dq_j}{2\pi\hbar} \tag{25}$$

which defines the integration measure. The functions, or *configurations*, $(q(t), p(t))$ must satisfy the initial and final conditions

$$q(t_i) = q_i, \qquad q(t_f) = q_f \tag{26}$$

Thus the matrix element $\langle q_f, t_f | q_i, t_i \rangle$ is expressible as a sum over histories in *phase space*. The weight of each history is the exponential factor of Eq. 24. Notice that the quantity in brackets it is just the Lagrangian

$$L = p\dot{q} - H(p, q) \tag{27}$$

Thus the matrix element is just

$$\langle q_f, t_f | q, t \rangle = \int \mathcal{D}p\mathcal{D}q \; e^{iS(q,p)/\hbar} \tag{28}$$

where $S(q, p)$ is the action of each history $(q(t), p(t))$. Also notice that the sum (or integral) runs over *independent* functions $q(t)$ and $p(t)$ which are not required to satisfy any constraint (apart from the initial and final conditions) and, in particular they are not the solution of the equations of motion. Expressions of these type are known as *path-integrals*. They are also called functional integrals, since the integration measure is a sum is over *functions*, instead of numbers as in a conventional integral.

Using a Gaussian integral of the form (which involves an analytic continuation)

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \; e^{i(p\dot{q} - \frac{p^2}{2m})\frac{\Delta t}{\hbar}} = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \; e^{i\frac{\Delta t}{2\hbar}\dot{q}^2} \tag{29}$$

we can integrate out explicitly the momenta in the path-integral and find a formula that involves only the histories of the coordinate alone. (Notice that there are no initial and final conditions on the momenta since the initial and final states have well defined positions.) The result is

$$\langle q_f, t_f | q_i, t_i \rangle = \int \mathcal{D}q \;\; e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt \; L(q, \dot{q})} \tag{30}$$

which is known as the *Feynman* Path Integral. Here $L(q, \dot{q})$ is

$$L(q, \dot{q}) = \frac{1}{2} m\dot{q}^2 - V(q) \tag{31}$$

and the sum over histories $q(t)$ is restricted by the boundary conditions $q(t_i) = q_i$ and $q(t_f) = q_f$.

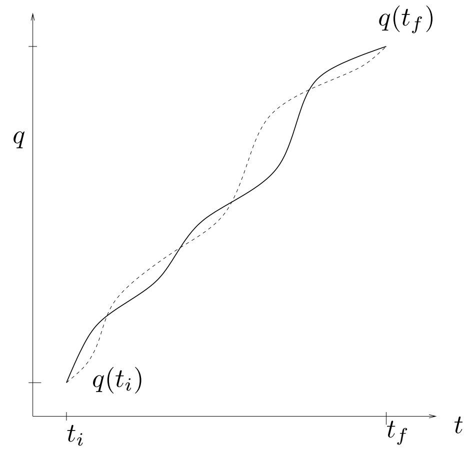


Figure 2: Two histories with the same initial and final states.

Notice now that the Feynman path-integral tells us that in the correspondence limit $\hbar \to 0$, the action S must be stationary since otherwise the contributions of the rapidly oscillating exponential will add up to zero. In other words, in the classical limit there is only one history $q_c(t)$ that contributes. For this history, $q_c(t)$, the action S is stationary, $\delta S = 0$, and $q_c(t)$ is the solution of the Classical Equation of Motion

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} \tag{32}$$

In other terms, in the correspondence limit $\hbar \to 0$, the evaluation of the Feynman path integral reduces to the requirement that the Least Action Principle should hold. We are in the classical limit.

5.2 Evaluating Path Integrals in Quantum Mechanics

Let us first discuss the following problem. We wish to know how to compute the amplitude $\langle q_f, t_f | q_i, t_i \rangle$ for a dynamical system whose Lagrangian has the standard form of Eq. 31. For simplicity we will begin with a linear harmonic oscillator.

The Hamiltonian for a linear harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 \tag{33}$$

and the associated Lagrangian is

$$L = \frac{m}{2}\dot{q}^2 - \frac{m\omega^2}{2} q^2 \tag{34}$$

Let $q_c(t)$ be the classical trajectory. It is the solution of the classical equations of motion

$$\frac{d^2 q_c}{dt^2} + \omega^2 q_c = 0 \tag{35}$$

Let us denote by $q(t)$ an arbitrary history of the system and by $\xi(t)$ its deviation from the classical solution $q_c(t)$. Since all the histories, including the classical trajectory $q_c(t)$, obey the *same* initial and final conditions

$$q(t_i) = q_i \qquad q(t_f) = q_f \tag{36}$$

it follows that $\xi(t)$ obeys instead *vanishing* initial and final conditions:

$$\xi(t_i) = \xi(t_f) = 0 \tag{37}$$

After some trivial algebra it is easy to show that the action S for an arbitrary history $q(t)$ has the property

$$S(q,\dot{q}) = S(q_c,\dot{q}_c) + S(\xi,\dot{\xi}) + \int_{t_i}^{t_f} dt\, \frac{d}{dt}\left[m\xi \frac{dq_c}{dt}\right] + \int_{t_i}^{t_f} dt\; m\xi \left(\frac{d^2 q_c}{dt^2} + \omega^2 q_c\right) \tag{38}$$

The third term vanishes due to the boundary conditions on ξ, Eq. 37, and the last term also vanishes since q_c is a solution of the classical equation of motion Eq. 35. These two features hold for all systems, even if they are not harmonic. However, the Lagrangian (and hence the action) for ξ, the second term in Eq. 38, in general is not the same as the action for the classical trajectory (the first term). Only for the harmonic oscillator $S(\xi,\dot{\xi})$ has the same form as $S(q_c,\dot{q}_c)$.

Hence, for a harmonic oscillator we get

$$\langle q_f, t_f | q_i, t_i \rangle = e^{iS(q_c,\dot{q}_c)/\hbar} \int_{\xi(t_i)=\xi(t_f)=0} \mathcal{D}\xi\, e^{(i/\hbar)\int_{t_i}^{t_f} dt L(\xi,\dot{\xi})} \tag{39}$$

Notice that the information on the initial and final states enters only through the factor associated with the classical trajectory. For the linear harmonic oscillator, the quantum mechanical contribution is independent of the initial and final states. Thus, we need to do two things: 1) we need an explicit solution $q_c(t)$ of the equation of motion, for which we will compute $S(q_c,\dot{q}_c)$, and 2) we need to compute the quantum mechanical correction, the last factor in Eq. 39, which measures the strength of the quantum fluctuations.

For a general dynamical system, whose Lagrangian has the form of Eq. 31, the action of Eq. 38 takes the form

$$\begin{aligned} S(q,\dot{q}) &= S(q_c,\dot{q}_c) + S_{\text{eff}}(\xi,\dot{\xi};q_c) \\ &\quad + \int_{t_i}^{t_f} dt\, \frac{d}{dt}\left[m\xi \frac{dq_c}{dt}\right] + \int_{t_i}^{t_f} dt\, \left(m\frac{d^2 q_c}{dt^2} + \left.\frac{\partial V}{\partial q}\right|_{q_c}\right)\xi(t) \end{aligned} \tag{40}$$

where the effective Lagrangian $L_{\text{eff}}(\xi, \dot{\xi}; q_c)$ is

$$L_{\text{eff}}(\xi, \dot{\xi}) = \frac{1}{2} m \dot{\xi}^2 - \frac{1}{2} \left. \frac{\partial^2 V}{\partial q^2} \right|_{q_c} \xi^2 - O(\xi^3) \tag{41}$$

Once again, the boundary conditions $\xi(t_i) = \xi(t_f) = 0$ and the fact the $q_c(t)$ is a solution of the equation of motion together imply that the last two terms of Eq. 40 vanish identically.

Thus, to the extent that we are allowed to neglect $O(\xi^3)$ the corrections, the effective Lagrangian L_{eff} can be approximated by a Lagrangian which is quadratic in the fluctuation ξ. In general, the effective Lagrangian will depend on the actual classical trajectory, since $V^{''}(q_c)$ in general is not a constant, but a function of time determined by $q_c(t)$. However, if one is interested in the quantum fluctuations about a *minimum* of the potential $V(q)$, then $q_c(t)$ is constant (and equal to the minimum). We will discuss below this case in detail.

Before we embark in an actual computation it is worthwhile to ask when should the neglecting of the $O(\xi^3)$ terms be a good approximations. Since we are expanding about the classical path q_c, we expect that this approximation should be correct as we formally take the limit $\hbar \to 0$. In the path integral the effective action always appears in the combination $S_{\text{eff}}/\hbar$. Hence, for an effective action which is quadratic in ξ, we can eliminate the dependence on $\hbar$ by the rescaling

$$\xi = \sqrt{\hbar} \tilde{\xi} \tag{42}$$

This rescaling leaves the classical contribution $S(q_c)/\hbar$ unaffected. However, terms with higher powers in ξ, say $O(\tilde{\xi}^n)$, scale like $\hbar^{n/2}$. Thus the action (divided by $\hbar$) has an expansion of the form

$$\frac{S}{\hbar} = \frac{1}{\hbar} S^{(0)}(q_c) + S^{(2)}(\tilde{\xi}; q_c) + \sum_{n=3}^{\infty} \hbar^{n/2} S^{(n)}(\tilde{\xi}; q_c) \tag{43}$$

Thus, in the limit $\hbar \to 0$, we can expand the weight of the path integral in powers of $\hbar$. The matrix element we are calculating then takes the form

$$\langle q_f, t_f | q_i, t_i \rangle = e^{i S^{(0)}(q_c)/\hbar} \ \mathcal{Z}^{(2)}(q_c) \ \left(1 + O(\hbar)\right) \tag{44}$$

The quantity $\mathcal{Z}^{(2)}(q_c)$ is the result of keeping only the quadratic approximation. The higher order terms are a power series expansion in $\hbar$ and are analytic in $\hbar$. (Here I have used the fact that by symmetry the odd powers in ξ in general do not contribute, although there are some cases where they do.)

Let us now calculate the effect of the quantum fluctuations to quadratic order. This is the WKB approximation. Let us denote this factor by $\mathcal{Z}$,

$$\mathcal{Z}^{(2)}(q_c) = \int_{\tilde{\xi}(t_i) = \tilde{\xi}(t_f) = 0} \mathcal{D}\xi \ e^{i \int_{t_i}^{t_f} dt \ L_{\text{eff}}^{(2)}(\tilde{\xi}, \dot{\tilde{\xi}}; q_c)} \tag{45}$$

It is elementary to show that, due to the boundary conditions, the action $S_{\text{eff}}(\xi, \dot{\xi})$ becomes

$$S_{\text{eff}}(\tilde{\xi}, \dot{\tilde{\xi}}) = \frac{1}{2} \int_{t_i}^{t_f} dt \ \tilde{\xi}(t) \ \left[-m \frac{d^2}{dt^2} - V^{''}(q_c(t)) \right] \tilde{\xi}(t) \tag{46}$$

The differential operator

$$\hat{A} = -m\frac{d^2}{dt^2} - V^{''}(q_c(t)) \tag{47}$$

has the form of a Schrödinger operator for a particle on a "coordinate" t in a potential $-V^{''}(q_c(t))$.

Let $\psi_n(t)$ be a complete set of eigenfunctions of $\hat{A}$ satisfying the boundary conditions $\psi(t_i) = \psi(t_f) = 0$. Completeness and othonormality implies that the eigenfunctions $\{\psi_n(t)\}$ satisfy

$$\begin{aligned} \sum_n \psi_n^*(t)\psi_n(t') &= \delta(t-t') \\ \int_{t_i}^{t_f} dt\; \psi_n^*(t)\psi_m(t) &= \delta_{n,m} \end{aligned} \tag{48}$$

We can expand $\tilde{\xi}(t)$ as a linear combination of the eigenfunctions $\{\psi_n(t)\}$,

$$\xi(t) = \sum_n c_n \psi_n(t) \tag{49}$$

Clearly, we have $\tilde{\xi}(t_i) = \tilde{\xi}(t_f) = 0$ as we should.

For the special case of $q_i = q_f = q_0$, where q_0 is a minimum of the potential $V(q)$, $V''(q_0) = \omega_{\text{eff}} > 0$ is a constant, and the eigenvectors of the Schrödinger operator are just plane waves. (For a linear harmonic oscillator $\omega_{\text{eff}} = \omega$.) Thus, in this case the eigenvectors are

$$\psi_n(t) = b_n \sin(k_n(t - t_i)) \tag{50}$$

where

$$k_n = \frac{\pi n}{t_f - t_i} \qquad n = 1, 2, 3, \ldots \tag{51}$$

and $b_n = 1/\sqrt{t_f - t_i}$. The eigenvalues of $\hat{A}$ are

$$A_n = k_n^2 - \omega_{\text{eff}}^2 = \frac{\pi^2}{(t_f - t_i)^2} n^2 - \omega_{\text{eff}}^2 \tag{52}$$

By using the expansion of Eq. 49, we find that the action $S^{(2)}$ takes the form

$$S^{(2)} = \frac{1}{2}\int_{t_i}^{t_f} dt\; \tilde{\xi}(t)\; \hat{A}\; \tilde{\xi}(t) = \frac{1}{2}\sum_n A_n c_n^2 \tag{53}$$

where we have used the completeness and orthonormality of the basis functions $\{\psi_n(t)\}$. Furthermore, the expansion is a canonical transformation $\tilde{\xi}(t) \to c_n$. More to the point, the expansion is actually a *parametrization* of the possible histories in terms of a set of orthonormal functions, and it can be used to define the integration measure to be

$$\mathcal{D}\tilde{\xi} = \mathcal{N} \prod_n \frac{dc_n}{\sqrt{2\pi}} \tag{54}$$

with unit Jacobian. Here $\mathcal{N}$ is an irrelevant normalization constant that will be defined below.

Finally, the (formal) Gaussian integral (defined by a suitable analytic continuation)

$$\int_{-\infty}^{\infty} \frac{dc_n}{\sqrt{2\pi}} \, e^{(i/2)A_n c_n^2} = [-iA_n]^{-1/2} \tag{55}$$

can be used to write the amplitude as

$$\mathcal{Z}^{(2)} = \mathcal{N} \prod_n A_n^{-1/2} \equiv \mathcal{N} \, (\text{Det}\hat{A})^{-1/2} \tag{56}$$

where we have used the *definition* that the determinant of an *operator* is equal to the product of its eigenvalues. Therefore, up to a normalization constant, $\mathcal{Z}^{(2)} = (\text{Det}\hat{A})^{-1/2}$. We have thus reduced the problem of the computation of the leading (Gaussian) fluctuations to the path-integral to the computation of a determinant of the fluctuation operator, a differential operator defined by the choice of classical trajectory. Below you will see how this is done.

It is useful to consider the related problem obtained by an analytic continuation to *imaginary time*, $t \to -i\tau$. We saw before that there is a relation between this situation and Statistical Physics. We will now work out one example that will be very instructive.

Formally, upon the analytic continuation $t \to -i\tau$ we get

$$\langle q_f| \exp\left(\frac{i}{\hbar} H(t_f - t_i)\right) |q_i\rangle \to \langle q_f| \exp\left(-\frac{1}{\hbar} H(\tau_f - \tau_i)\right) |q_i\rangle \tag{57}$$

Let us choose

$$\tau_i = 0 \qquad \tau_f = \beta\hbar \tag{58}$$

where $\beta = 1/T$, and T is the temperature (in units of $k_B = 1$). Hence, we find that

$$\langle q_f, -i\beta/\hbar | q_i, 0\rangle = \langle q_f| e^{-\beta H} |q_i\rangle \tag{59}$$

The operator $\hat{\rho}$

$$\hat{\rho} = e^{-\beta H} \tag{60}$$

is the *Density Matrix* in the Canonical Ensemble of Statistical Mechanics for a system with Hamiltonian H in thermal equilibrium at temperature T.

It is customary to define the *Partition Function* $\mathcal{Z}$,

$$\mathcal{Z} = \text{tr} e^{-\beta H} \equiv \int dq \, \langle q| e^{-\beta H} |q\rangle \tag{61}$$

where I inserted a complete set of eigenstates of $\hat{Q}$. Using the results that were derived above, we see that the partition function $\mathcal{Z}$ can be written as a *Feynman path integral in imaginary time*, of the form

$$\begin{aligned}\mathcal{Z} &= \int \mathcal{D}q[\tau] \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \;\left[\frac{1}{2}m\left(\frac{\partial q}{\partial \tau}\right)^2 + V(q)\right]\right\} \\ &\equiv \int \mathcal{D}q[\tau] \exp\left\{-\int_0^{\beta} d\tau \;\left[\frac{m}{2\hbar^2}\left(\frac{\partial q}{\partial \tau}\right)^2 + V(q)\right]\right\}\end{aligned} \tag{62}$$

where, in the last equality we have rescaled $\tau \to \tau/\hbar$. Eq. 62 is known as the *Feynman-Kac Formula*.

Since the Partition Function is a *trace* over states, we must use boundary conditions such that the initial and final states are the same state, and to do a sum over all such states. In other terms, we must have *periodic* boundary conditions in imaginary time (PBC's),*i.e.,*

$$q(\tau) = q(\tau + \beta) \tag{63}$$

Therefore a quantum mechanical system at finite temperature T can be described in terms of an equivalent system in classical statistical mechanics with Hamiltonian (or energy)

$$\mathcal{H} = \frac{m}{2\hbar^2}\left(\frac{\partial q}{\partial \tau}\right)^2 + V(q) \tag{64}$$

on a segment of length $1/T$ and obeying PBC's. This effectively means that the segment is actually a ring of length $\beta = 1/T$.

Alternatively, upon inserting a complete set of eigenstates of the Hamiltonian, it is easy to see that an arbitrary matrix element of the density matrix has the form

$$\begin{aligned}\langle q'|e^{-\beta H}|q\rangle &= \sum_{n=0}^{\infty}\langle q'|n\rangle\langle n|q\rangle e^{-\beta E_n} \\ &= \sum_{n=0}^{\infty} e^{-\beta E_n}\psi_n^*(q')\psi_n(q) \;\xrightarrow[\beta \to \infty]{}\; e^{-\beta E_0}\psi_0^*(q')\psi_0(q)\end{aligned} \tag{65}$$

where $\{E_n\}$ are the eigenvalues of the Hamiltonian, E_0 is the ground state energy and $\psi_0(q)$ is the ground state wave function.

Therefore, we can calculate both the ground state energy E_0 and the ground state wave function from the density matrix and consequently from the (imaginary time) path integral.For example, from the identity

$$E_0 = -\lim_{\beta\to\infty}\frac{1}{\beta}\ln \mathrm{tr} e^{-\beta H} \tag{66}$$

we see that the ground state energy is given by

$$E_0 = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln \int_{q(0)=q(\beta)} \mathcal{D}q \; \exp\left\{ -\int_0^\beta d\tau \; \left[\frac{m}{2\hbar^2} \left(\frac{\partial q}{\partial \tau}\right)^2 + V(q) \right] \right\} \tag{67}$$

Mathematically, the imaginary time path integral is a better behaved object than its real time counterpart, since it is a sum of positive quantities, the statistical weights. In contrast, the Feynman path integral (in real time) is a sum of phases and as such it is an ill-defined object. It is actually conditionally convergent and to make sense of it a number of convergence factors (or regulators) will have to be introduced. The effect of these convergence factors is actually an analytic continuation to imaginary time. We will encounter the same problem in the calculation of propagators. Thus, the imaginary time path integral, often referred to as the Euclidean path integral (as opposed to Minkowski), can be used to describe both a quantum system and a statistical mechanics system.

Finally, we notice that at low temperatures $T \to 0$, the Euclidean Path Integral can be approximated using methods similar to the ones we discussed for the (real time) Feynman Path Integral. The main difference is that we must sum over trajectories which are periodic in imaginary time with period $\beta = 1/T$. In practice this sum can only be done exactly for simple systems such as the harmonic oscillator, and for more general systems one has to resort to some form of perturbation theory. Here we will consider a physical system described by a dynamical variable q and a potential energy $V(q)$ which has a minimum at $q_0 = 0$. For simplicity we will take $V(0) = 0$ and we will denote by $m\omega^2 = V^{''}(0)$ (in other words, an effective harmonic oscillator). The partition function is given by the Euclidean path integral

$$\mathcal{Z} = \int \mathcal{D}q[\tau] \exp\left\{ -\frac{1}{2} \int_0^\beta \xi(\tau) \hat{A}_E \xi(\tau) d\tau \right] \tag{68}$$

where $\hat{A}_E$ is the imaginary time, or Euclidean, version of the operator $\hat{A}$, and it is given by

$$\hat{A}_E = -\frac{m}{\hbar^2} \frac{d^2}{d\tau^2} + V^{''}(q_c(\tau)) \tag{69}$$

The functions this operator acts on obey periodic boundary conditions with period β. Notice the important change in the sign of the term of the potential. Hence, once again we will need to compute a functional determinant, although the operator now acts on functions obeying periodic boundary conditions. In Physics 582 we will see that in the case of *fermionic* theories, the boundary conditions become *antiperiodic*.

5.2.1 Computation of the Functional Determinant

We will now do the computation of the determinant in $\mathcal{Z}^{(2)}$. We will do the calculation in imaginary time and then we will carry out the analytic continuation to real time. We want to compute

$$D = \mathrm{Det}\left[-\frac{m}{\hbar^2}\frac{d^2}{d\tau^2} + V^{''}(q_c(\tau))\right] \tag{70}$$

subject to the requirement that the space of functions that the operator acts on obeys specific boundary conditions in (imaginary) time. We will be interested in two cases: (a) Vanishing Boundary Conditions (VBC's), which are useful to study quantum mechanics at $T = 0$, and (b) Periodic Boundary Conditions (PBC's) with period $\beta = 1/T$. The approach is somewhat different in the two situations.

1. Vanishing Boundary Conditions:
   This method is explained in detail in Sidney Coleman's book, *Aspects of Symmetry*. I will follow his approach closely.

   We define the (real) variable $x = \frac{\hbar}{m}\tau$. The range of x is the interval $[0, L]$, with $L = \hbar\beta/\sqrt{m}$. Let us consider the following eigenvalue problem for the Schrödinger operator $-\partial^2 + W(x)$, *i.e.,*

   $$\left(-\partial^2 + W(x)\right)\psi(x) = \lambda\psi(x) \tag{71}$$

   subject to the boundary conditions $\psi(0) = \psi(L) = 0$. Formally, the determinant is given by

   $$D = \prod_n \lambda_n \tag{72}$$

   where $\{\lambda_n\}$ is the spectrum of eigenvalues of the operator $-\partial^2 + W(x)$ for a space of functions satisfying a given boundary condition.

   Let us define an auxiliary function $\psi_\lambda(x)$, with λ a real number not necessarily in the spectrum of the operator, such that the following requirements are met:

   (a) $\psi_\lambda(x)$ is a solution of Eq. 71, and

   (b) ψ_λ obeys the *initial* conditions, $\psi_\lambda(0) = 0$ and $\partial_x\psi_\lambda(0) = 1$.

   It is easy to see that $-\partial^2 + W(x)$ has an eigenvalue at λ_n if and only if $\psi_{\lambda_n}(L) = 0$. (Because of this property this procedure is known as the Shooting Method.) Hence, the determinant D of Eq. 72 is equal to the product of the *zeros* of $\psi_\lambda(x)$ at $x = L$.

   Consider now two potentials $W^{(1)}$ and $W^{(2)}$, and the associated functions, $\psi_\lambda^{(1)}(x)$ and $\psi_\lambda^{(2)}(x)$. Let us show that

   $$\mathrm{Det}\left[\frac{-\partial^2 + W^{(1)}(x) - \lambda}{-\partial^2 + W^{(2)}(x) - \lambda}\right] = \frac{\psi_\lambda^{(1)}(L)}{\psi_\lambda^{(2)}(L)} \tag{73}$$

   The l. h. s. of Eq. 73 is a meromorphic function of λ in the complex plane, which has simple zeros at the eigenvalues of $-\partial^2 + W^{(1)}(x)$ and simple poles at the eigenvalues of $-\partial^2 + W^{(2)}(x)$. Also, the l. h. s. of Eq. 73 approaches 1 as $|\lambda| \to \infty$, except along the positive real axis which is where the spectrum of eigenvalues of both operators is. Here we have assumed that the eigenvalues of the operators are non-degenerate, which is the general case. Similarly, the r. h. s. of Eq. 73 is also a meromorphic function of λ, which has *exactly the same zeros and the same poles* as the l. h. s. . It also goes to 1 as $|\lambda| \to \infty$ (again, except along the positive real axis), since the wave-functions ψ_λ are asymptotically plane waves in this limit . Therefore, the function formed by taking the ratio r. h. s. / l. h. s. is an *analytic* function on the *entire complex plane* and it approaches 1 as $|\lambda| \to \infty$. Then, general theorems of the Theory of Functions of a Complex Variable tell us that this function is *equal* to 1 everywhere.

From these considerations we conclude that the following ratio is independent of $W(x)$,

$$\frac{\text{Det}\left(-\partial^2 + W(x) - \lambda\right)}{\psi_\lambda(L)} \tag{74}$$

We now define a constant $\mathcal{N}$ such that

$$\frac{\text{Det}\left(-\partial^2 + W(x)\right)}{\psi_0(L)} = \pi\hbar\mathcal{N}^2 \tag{75}$$

Then, we can write

$$\mathcal{N}\left[\text{Det}\left(-\partial^2 + W\right)\right]^{-1/2} = \left[\pi\hbar\psi_0(L)\right]^{-1/2} \tag{76}$$

Thus we reduced the computation of the determinant (including the normalization constant) to finding the function $\psi_0(L)$. For the case of the linear harmonic oscillator, this function is the solution of

$$\left[-\frac{\partial^2}{\partial x^2} + m\omega^2\right]\psi_0(x) = 0 \tag{77}$$

with the initial conditions, $\psi_0(0) = 0$ and $\psi_0'(0) = 1$. The solution is

$$\psi_0(x) = \frac{1}{\sqrt{m}\omega}\sinh(\sqrt{m}\omega x) \tag{78}$$

Hence,

$$\mathcal{Z} = \mathcal{N}\left[\text{Det}\left(-\frac{\partial^2}{\partial x^2} + m\omega^2\right)\right]^{-1/2} = \left[\pi\hbar\psi_0(L)\right]^{-1/2} \tag{79}$$

and we find

$$\mathcal{Z} = \left[\frac{\pi\hbar}{\sqrt{m}\omega}\sinh(\beta\omega)\right]^{-1/2} \tag{80}$$

where we have used $L == \hbar\beta/\sqrt{m}$. From this result we find that the ground state energy is

$$E_0 = \lim_{\beta\to\infty}\frac{-1}{\beta}\ln\mathcal{Z} = \frac{\hbar\omega}{2} \tag{81}$$

as it should be.

Finally, by means of an analytic continuation back to real time, we can use these results to find, for instance, the amplitude to return to the origin after some time T. Thus, for $t_f - t_i = T$ and $q_f = q_i = 0$, we get

$$\langle 0, T|0, 0\rangle = \left[\frac{i\pi\hbar}{\sqrt{m}\omega}\sin(\omega T)\right]^{-1/2} \tag{82}$$

2. Periodic Boundary Conditions:
Periodic boundary conditions imply that the histories satisfy $q(\tau) = q(\tau + \beta)$. Hence, these functions can be expanded in a Fourier series of the form

$$q(\tau) = \sum_{n=-\infty}^{\infty} e^{i\omega_n\tau} q_n \tag{83}$$

where $\omega_n = 2\pi n/\beta$. Since $q(\tau)$ is real, we have the constraint $q_{-n} = q_n^*$. For such configurations (or histories) the action becomes

$$\begin{aligned} S &= \int_0^\beta d\tau \left[\frac{m}{2\hbar^2}\left(\frac{\partial q}{\partial\tau}\right)^2 + \frac{1}{2}V^{''}(0)q^2\right] \\ &= \frac{\beta}{2}V^{''}(0)q_0^2 + \frac{\beta}{2}\sum_{n\geq 1}\left[\frac{m}{\hbar^2}\omega_n^2 + V^{''}(0)\right]|q_n|^2 \end{aligned} \tag{84}$$

The integration measure now is

$$\mathcal{D}q[\tau] = \mathcal{N}\frac{dq_0}{\sqrt{2\pi}}\prod_{n\geq 1}\frac{d\text{Re}q_n\; d\text{Im}q_n}{2\pi} \tag{85}$$

where $\mathcal{N}$ is a normalization constant that will be discussed below. After doing the Gaussian integrals, the partition function becomes,

$$\mathcal{Z} = \mathcal{N}\frac{1}{\sqrt{\beta V''(0)}}\prod_{n\geq 1}\frac{1}{\frac{\beta m}{\hbar^2}\omega_n^2 + \beta V''(0)} = \mathcal{N}\left[\prod_{n=-\infty}^{\infty}\frac{1}{\frac{\beta m}{\hbar^2}\omega_n^2 + \beta V''(0)}\right]^{1/2} \tag{86}$$

Formally, the infinite products that enter in this equation are divergent. The normalization constant $\mathcal{N}$ eliminates this divergence. This is an example of what is called a *regularization*. The regularized partition function is

$$\mathcal{Z} = \sqrt{\frac{m}{\hbar^2\beta}}\frac{1}{\sqrt{\beta V''(0)}}\prod_{n\geq 1}\left[1 + \frac{\hbar^2 V^{''}(0)}{m\omega_n^2}\right]^{-1} \tag{87}$$

Using the identity

$$\prod_{n\geq 1}\left(1 + \frac{a^2}{n^2\pi^2}\right) = \frac{a}{\sinh a} \tag{88}$$

we find

$$\mathcal{Z} = \frac{1}{2\sinh\left(\frac{\beta\hbar}{2}\left(\frac{V''(0)}{m}\right)^{1/2}\right)} \tag{89}$$

which is the standard partition function for a linear harmonic oscillator, see L. D. Landau and E. M. Lifshitz, *Statistical Physics*.

5.3 Path Integrals for a Scalar Field Theory

We will now develop the path-integral quantization picture for a scalar field theory. Our starting point will be the canonically quantized scalar field. As we saw before in canonical quantization the scalar field $\hat{\phi}(x)$ is an operator that acts on a Hilbert space of states. We will use the field representation, which is the analog of the conventional coordinate representation in Quantum Mechanics. Thus, the basis states are labelled by the field configuration at some fixed time x_0, *i.e.,* a set of states of the form $\{\ |\{\phi(\vec{x}, x_0)\}\rangle\ \}$. The field operator $\hat{\phi}(\vec{x}, x_0)$ acts trivially on these states,

$$\hat{\phi}(\vec{x}, x_0)|\{\phi(\vec{x}, x_0)\}\rangle = \phi(\vec{x}, x_0)|\{\phi(\vec{x}, x_0)\}\rangle \tag{90}$$

The set of states $\{\ |\{\phi(\vec{x}, x_0)\}\rangle\ \}$ is both complete and orthonormal. Completeness here means that these states span the entire Hilbert space. Consequently the identity operator $\hat{\mathcal{I}}$ in the full Hilbert space can be expanded in a complete basis in the usual manner, which for this basis it means

$$\hat{\mathcal{I}} = \int \mathcal{D}\phi(\vec{x}, x_0)\ |\{\phi(\vec{x}, x_0)\}\rangle\langle\{\phi(\vec{x}, x_0)\}| \tag{91}$$

Notice that since the completeness condition involves a sum over all the states in the basis and since this basis is the set of field configurations at a given time x_0, we will need to give a definition for integration measure which represents the sums over the field configurations. In this case there is a trivial definition,

$$\mathcal{D}\phi(\vec{x}, x_0) = \prod_{\vec{x}} d\phi(\vec{x}, x_0) \tag{92}$$

Likewise, othonormality of the basis states is the condition

$$\langle\phi(\vec{x}, x_0)|\phi'(\vec{x}, x_0)\rangle = \prod_{\vec{x}} \delta\left(\phi(\vec{x}, x_0) - \phi'(\vec{x}, x_0)\right) \tag{93}$$

Thus, we have a working definition of the Hilbert space for a real scalar field. Naturally, there are many other definitions of this Hilbert space and they are all equally good.

We saw in the previous section that in canonical quantization the classical canonical momentum $\Pi(\vec{x}, x_0)$, defined as

$$\Pi(\vec{x}, x_0) = \frac{\delta\mathcal{L}}{\delta\partial_0\phi(\vec{x}, x_0)} = \partial_0\phi(\vec{x}, x_0) \tag{94}$$

becomes an operator that acts on the same Hilbert space as the field itself ϕ does. The field ϕ and the canonical momentum π satisfy *equal time canonical commutation relations* (CCR)

$$\left[\hat{\phi}(\vec{x}, x_0), \hat{\Pi}(\vec{y}, x_0)\right] = i\hbar\delta^3(\vec{x} - \vec{y}) \tag{95}$$

Here we will use the Lagrangian density for a real scalar field

$$\mathcal{L} = \frac{1}{2}\left(\partial_\mu \phi\right)^2 - V(\phi) \tag{96}$$

It is a simple matter to generalize what follows below to more general cases, such as complex fields and/or several components. Let us also recall that the Hamiltonian for a scalar field is given by

$$\hat{H} = \int d^3x \left[\frac{\hat{\Pi}^2}{2} + \frac{1}{2}\left(\vec{\bigtriangledown}\hat{\phi}\right)^2 + V(\hat{\phi})\right] \tag{97}$$

For reasons that will become clear soon, it is convenient to add an extra term to the Lagrangian density of the scalar field, Eq. 96, of the form

$$\mathcal{L}_{\text{source}} = J(x)\ \phi(x) \tag{98}$$

The field $J(x)$ is called an *external source* and represents the effects of external sources on the scalar field. The field $J(x)$ is the analog of external *forces* acting on a system of classical particles. Here we will always assume that the sources $J(x)$ vanish both at spacial infinity (at all times) and everywhere in both the remote past and in the remote future,

$$\lim_{|\vec{x}|\to\infty} J(\vec{x}, x_0) = 0 \qquad \lim_{x_0\to\pm\infty} J(\vec{x}, x_0) = 0 \tag{99}$$

The total Lagrangian density is

$$\mathcal{L}(\phi, J) = \mathcal{L} + \mathcal{L}_{\text{source}} \tag{100}$$

Notice that since the source $J(x)$ is generally a function of space and time, the Hamiltonian that follows from this Lagrangian is formally time-dependent.

We will derive the path integral for this quantum field theory by following the same procedure we used for the case of a finite quantum mechanical system. Hence we begin by considering the amplitude

$${}_J\langle\{\phi(\vec{x}, x_0)\}|\{\phi'(\vec{y}, y_0)\}\rangle_J \tag{101}$$

In other words, we want the amplitude in the background of the sources $J(x)$. We will be interested in situations in which x_0 is in the remote future and y_0 is in the remote past. It turns out that this amplitude is intimately related to the computation of ground state (or *vacuum*) expectation values of *time ordered* products of field operators in the Heisenberg representation

$$G^{(N)}(x_1, \ldots, x_N) \equiv \langle 0|T[\hat{\phi}(x_1)\ldots\hat{\phi}(x_N)]|0\rangle \tag{102}$$

which are the N-point *Green Functions*. In particular the 2-point function

$$G^{(2)}(x_1,\dots,x_N)\equiv\langle 0|T[\hat\phi(x_1)\hat\phi(x_2)]|0\rangle \tag{103}$$

is known as the *Feynman Propagator* for this theory. We will see later on that all quantities of physical interest can be obtained from a suitable Green function of the type of Eq. 102.

In Eq. 102 we have use the notation $T[\hat\phi(x_1)\dots\hat\phi(x_N)]$ for the *time-ordered product* of Heisenberg field operators. For *any* pair Heisenberg of operators $\hat A(\vec x,x_0)$ and $\hat B(\vec y,y_0)$, (which commute for space-like separations) the time ordered product is defined to be

$$T[\hat A(\vec x,x_0)\hat B(\vec y,y_0)]=\theta(x_0-y_0)\hat A(\vec x,x_0)\hat B(\vec y,y_0)+\theta(y_0-x_0)\hat B(\vec y,y_0)\hat A(\vec x,x_0) \tag{104}$$

where $\theta(x)$ is the step (or Heaviside) function

$$\theta(x)=\begin{cases}1 & \text{if } x\geq 0,\\ 0 & \text{otherwise}\end{cases} \tag{105}$$

This definition is generalized by induction to any number of operators. Notice that inside a time-ordered product the Heisenberg operators behave as numbers.

Let us now recall the structure of the derivation that we gave of the path integral in Quantum Mechanics. We will paraphrase that derivation for this field theory. We considered an amplitude equivalent to Eq. 101, and realized that this amplitude is actually a matrix element of the evolution operator,

$$_J\langle\{\phi(\vec x,x_0)\}|\{\phi'(\vec y,y_0)\}\rangle_J=\langle\{\phi(\vec x)\}|T\ e^{-i\int_{y_0}^{x_0}dx_0'\ \hat H(x_0')/\hbar}|\{\phi'(\vec y)\}\rangle \tag{106}$$

where T stands for the time ordering symbol (not temperature!), and $H(x_0')$ is the time-dependent Hamiltonian:

$$H(x_0)=\int d^3x\left[\frac{1}{2}\Pi^2(\vec x,x_0)+\frac{1}{2}\left(\vec\nabla\phi(\vec x,x_0)\right)^2+V(\phi(\vec x,x_0))-J(\vec x,x_0)\right] \tag{107}$$

We then partitioned the time interval in a large number of steps of width Δt and inserted a complete set of eigenstates of the field operator $\hat\phi$, since it plays the role of the coordinate. As it turned out, we also had to insert complete sets of eigenstates of the canonical momentum operator, which here means the operator $\hat\Pi(\vec x)$. The result is the *phase-space* path integral

$$_J\langle\{\phi(\vec x,x_0)\}|\{\phi'(\vec y,y_0)\}\rangle_J=\int_{\text{b. c.}}\mathcal{D}\phi\mathcal{D}\Pi\ e^{\frac{i}{\hbar}\int_{y_0}^{x_0}dx_0'\left[\dot\phi\Pi-\mathcal{H}(\phi,\Pi)+J\phi\right]} \tag{108}$$

where b. c. indicates the boundary conditions required by the requirement that the initial and final states be $|\{\phi(\vec x,x_0)\}\rangle$ and $|\{\phi'(\vec y,y_0)\}\rangle$ respectively.

Exactly as in the case of the path integral for a particle, this theory has a Hamiltonian quadratic in the momenta $\Pi(x)$. Hence, we can further integrate out the field $\Pi(x)$, and obtain the Feynman path integral for the scalar field theory in the form of a *sum over histories* of field configurations:

$$
{}_J\langle\{\phi(\vec{x},x_0)\}|\{\phi'(\vec{y},y_0)\}\rangle_J = \mathcal{N}\int_{\text{b. c.}} \mathcal{D}\phi \; e^{\dfrac{i}{\hbar}S(\phi,\partial_\mu\phi,J)} \tag{109}
$$

where $\mathcal{N}$ is an (unimportant) normalization constant, and $S(\phi,\partial_\mu\phi,J)$ is the action for a real scalar field $\phi(x)$ coupled to a source $J(x)$,

$$
S(\phi,\partial_\mu\phi,J) = \int d^4x \, \left[\frac{1}{2}\left(\partial_\mu\phi\right)^2 - V(\phi) + J\phi\right] \tag{110}
$$

5.4 Path Integrals and Green Functions

In Quantum Field Theory we will be interested in calculating vacuum (*i. e.* ground state) expectation values of field operators at various space-time locations. Thus, instead of the amplitude ${}_J\langle\{\phi(\vec{x},x_0)\}|\{\phi'(\vec{y},y_0)\}\rangle_J$ we may be interested in a transition between an initial state, at $y_0 \to -\infty$ which is the *vacuum state* $|0\rangle$, *i.e.,* the ground state of the scalar field in the absence of the source $J(x)$, and a final state at $x_0 \to \infty$ which is also the vacuum state of the theory in the absence of sources. We will denote this matrix element by

$$
Z[J] = {}_J\langle 0|0\rangle_J \tag{111}
$$

This matrix element is called the *Vacuum Persistence Amplitude*.

Let us see now how the vacuum persistence amplitude is related to the Feynman path integral for a scalar field of Eq. 109. In order to do that we will assume that the source $J(x)$ is "on" between times $t < t'$ and that we watch the system on a much longer time interval $T < t < t' < T'$. For this interval, the amplitude is

$$
\begin{aligned}
{}_J\langle\{\Phi'(\vec{x},T')\}|\{\Phi(\vec{x},T)\}\rangle_J = & \int \mathcal{D}\phi(\vec{x},t)\;\mathcal{D}\phi'(\vec{x},t') \\
& \langle\{\Phi'(\vec{x},T')\}|\{\phi'(\vec{x},t')\}\rangle_J\langle\{\phi'(\vec{x},t')\}|\;\rangle\{\phi(\vec{x},t)\}_J\;\langle\{\phi(\vec{x},t)\}|\{\Phi(\vec{x},T)\}\rangle
\end{aligned} \tag{112}
$$

The matrix elements $\langle\{\Phi'(\vec{x},T')\}|\{\phi'(\vec{x},t')\}\rangle$ and $\langle\{\phi(\vec{x},t)\}|\{\Phi(\vec{x},T)\}\rangle$ are given by

$$
\begin{aligned}
\langle\{\phi(\vec{x},t)\}|\{\Phi(\vec{x},T)\}\rangle = & \sum_m \Psi_m[\{\phi(\vec{x})\}]\Psi_n^*[\{\Phi(\vec{x})\}]\; e^{-iE_n(t-T)/\hbar} \\
\langle\{\Phi'(\vec{x},T')\}|\{\phi'(\vec{x},t')\}\rangle \quad & \sum_n \Psi_n[\{\Phi'(\vec{x})\}]\Psi_n^*[\{\phi'(\vec{x})\}]\; e^{-iE_m(T'-t')/\hbar}
\end{aligned} \tag{113}
$$

where we have introduced complete sets of eigenstates $|\{\Psi_n\}\rangle$ of the Hamiltonian of the scalar field (without sources) and the corresponding wave functions, $\{\Psi_n(\Phi((\vec{x}))\}$.

We now analytically continue T along the *positive* imaginary time axis, and T' along the *negative* imaginary time axis, as shown in figure 3. After carrying

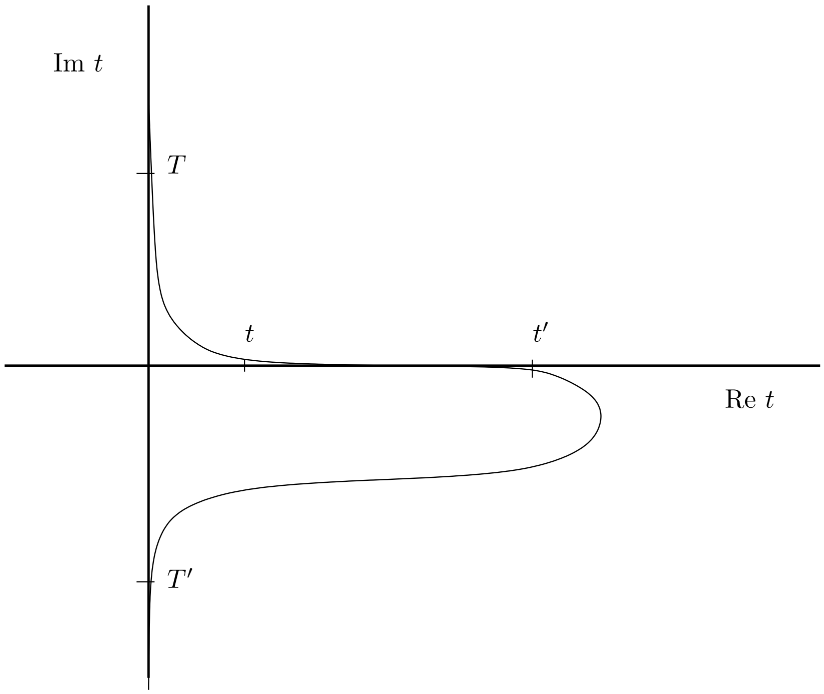


Figure 3: Analytic continuation

out the analytic continuation, we find that the following identities (essentially, the Gell-Mann-Low Theorem) hold,

$$\begin{aligned} \lim_{T\to+i\infty} e^{-iE_0T/\hbar}\langle\{\phi(\vec{x},t)\}|\{\Phi(\vec{x},T)\}\rangle &= \Psi_0[\{\phi\}]\ \Psi_0^*[\{\Phi\}]\ e^{-iE_0t/\hbar} \\ \lim_{T'\to-i\infty} e^{iE_0T'/\hbar}\langle\{\Phi'(\vec{x},T')\}|\{\phi(\vec{x},t')\}\rangle &= \Psi_0[\{\Phi'\}]\ \Psi_0^*[\{\phi'\}]\ e^{iE_0t'/\hbar} \end{aligned} \tag{114}$$

and all other terms drop out in this limit provided the vacuum state $|0\rangle$ is non-degenerate. Hence, in the same limit, we also find the following relation:

$$\lim_{T\to+i\infty}\lim_{T'\to-i\infty}\frac{\langle\{\Phi'(\vec{x},T')\}|\Phi(\vec{x},T)\}\rangle}{\exp\left[-iE_0(T'-T)/\hbar\right]\;\Psi_0^*[\{\Phi\}]\;\Psi_0[\{\Phi'\}]}$$
$$=\int\mathcal{D}\Phi\mathcal{D}\Phi'\;\Psi_0^*[\{\phi'(\vec{x},t')\}]\;\Psi_0[\{\phi(\vec{x},t)\}]\;{}_J\langle\{\phi'(\vec{x},t')\}|\{\phi(\vec{x},t)\}\rangle_J\;\equiv{}_J\langle 0|0\rangle_J \tag{115}$$

Eq. 115 gives us a relation between the Feynman Path Integral and the vacuum persistence amplitude of the form

$$Z[J]={}_J\langle 0|0\rangle_J=\mathcal{N}\lim_{T\to+i\infty}\lim_{T'\to-i\infty}\int\mathcal{D}\phi\;e^{\frac{i}{\hbar}\int_T^{T'}d^4x\;\left[\mathcal{L}(\phi,\partial_\mu\phi)+J\phi\right]} \tag{116}$$

In other words, in this asymptotically long time limit, the amplitude of Eq. 101 becomes identical to the vacuum persistence amplitude ${}_J\langle 0|0\rangle_J$, independently of the choice of the initial and final states.

Hence we find a direct relation between the vacuum persistence function $Z[J]$ and the Feynman Path Integral, given by Eq. 116. Notice that in this limit we can ignore the "hard" boundary condition and work instead with free boundary conditions. Or equivalently, physical properties become independent of the initial and final conditions placed. For these reasons, from now on we will write the simpler expression

$$Z[J]={}_J\langle 0|0\rangle_J=\mathcal{N}\int\mathcal{D}\phi\;e^{\frac{i}{\hbar}\int d^4x\;\left[\mathcal{L}(\phi,\partial_\mu\phi)+J\phi\right]} \tag{117}$$

This is a very useful relation. We will see now that $Z[J]$ is the generating function(al) of all the vacuum expectation values of time ordered products of fields, *i.e.* the Green functions. In particular, let us compute the expression

$$\frac{1}{Z[0]}\frac{\delta^2 Z[J]}{\delta J(x)\delta J(x')}\bigg|_{J=0}=\frac{1}{\langle 0|0\rangle}\frac{\delta^2\,{}_J\langle 0|0\rangle_J}{\delta J(x)\delta J(x')}\bigg|_{J=0}=\left(\frac{i}{\hbar}\right)^2\;\langle 0|T[\phi(x)\phi(x')]|0\rangle \tag{118}$$

Thus, the 2-point function, the *Feynman propagator* or *Green function* of the scalar field $\phi(x)$, $\langle 0|T[\phi(x)\phi(x')]|0\rangle$ becomes,

$$\langle 0|T[\phi(x)\phi(x')]|0\rangle=\frac{1}{\langle 0|0\rangle}\int\mathcal{D}\phi\;\phi(x)\;\phi(x')\;\exp\left(\frac{i}{\hbar}S[\phi,\partial_\mu\phi]\right) \tag{119}$$

Similarly, the N-point function $\langle 0|T[\phi(x_1)\dots\phi(x_N)]|0\rangle$ becomes

$$\begin{aligned}\langle 0|T[\phi(x_1)\dots\phi(x_N)]|0\rangle &= (-i\hbar)^N\;\frac{1}{\langle 0|0\rangle}\frac{\delta^N\,{}_J\langle 0|0\rangle_J}{\delta J(x_1)\dots\delta J(x_N)}\bigg|_{J=0}\\ &= \frac{1}{\langle 0|0\rangle}\int\mathcal{D}\phi\;\phi(x_1)\dots\phi(x_N)\;\exp\left(\frac{i}{\hbar}S[\phi,\partial_\mu\phi]\right)\end{aligned} \tag{120}$$

where

$$Z[0] = \langle 0|0\rangle = \int \mathcal{D}\phi \, \exp\left(\frac{i}{\hbar} S[\phi, \partial_\mu \phi]\right) \tag{121}$$

Therefore, we find that the Path Integral always yields vacuum expectation values of time-ordered products of operators. The quantity $Z[J]$ can thus be viewed as the generating functional of the Green functions of this theory. These are actually general results that hold for the path integrals of all theories.

5.5 Path Integrals in Euclidean Space and Statistical Physics

In the last section we saw how to relate the computation of transition amplitudes to path integrals in Minkowski space-time with specific boundary conditions dictated by the nature of the initial and final states. In particular we derived explicit expressions for the case of fixed boundary conditions. However we could have chosen other boundary conditions. For instance, for the amplitude to begin in any state at the initial time and to go back to the *same* state at the final time, but summing over all states. This is the same as to ask for the *trace*

$$\begin{aligned} Z'[J] = \int \mathcal{D}\Phi_J \langle \{\Phi(\vec{x}, t')\} | \{\Phi(\vec{x}, t)\}\rangle_J \equiv & \quad \mathrm{Tr}\, T\, e^{-\frac{i}{\hbar}\int d^4x\, (\mathcal{H} - J\phi)} \\ \equiv & \quad \int_{\mathrm{PBC}} \mathcal{D}\phi \;\; e^{\frac{i}{\hbar}\int d^4x\, (\mathcal{L} + J\phi)} \end{aligned} \tag{122}$$

where PBC stands for periodic boundary conditions on some generally *finite* time interval $t' - t$, and T is the time-ordering symbol.

Let us now carry the analytic continuation to imaginary time $t \to -i\tau$, *i.e.* a Wick Rotation. Upon a Wick rotation the theory has Euclidean invariance, *i.e.,* rotations and translations in $D = d+1$-dimensional space. Imaginary time plays the same role as the other d spacial dimensions. Hereafter we will denote imaginary time by x_D, and all vectors will have indices μ that run from 1 to D.

We will consider two cases: infinite imaginary time interval, and finite imaginary time interval.

5.5.1 Infinite Imaginary Time Interval

In this case the path integral becomes

$$Z'[J] = \int \mathcal{D}\phi \; e^{-\int d^Dx\, (\mathcal{L}_E - J\phi)} \tag{123}$$

where D is the total number of space-time dimensions. Here we are discussing the case $D = 4$, but it is obviously valid more generally. Here $\mathcal{L}_E$ is the Euclidean Lagrangian

$$\mathcal{L}_E = \frac{1}{2}(\partial_0 \phi)^2 + \frac{1}{2}(\vec{\bigtriangledown}\phi)^2 + V(\phi) \tag{124}$$

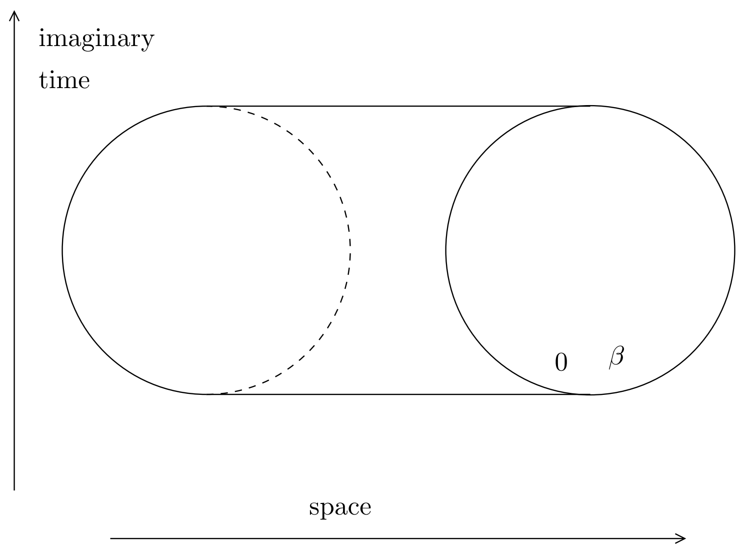


Figure 4: Periodic boundary conditions wraps space-time into a cylinder.

The path integral of Eq. 123 has two interpretations. One is simply the infinite time limit (in imaginary time) and therefore it must be identical to the vacuum persistence amplitude ${}_J\langle 0|0\rangle_J$. The only difference is that from here we get all the N-point functions in Euclidean space-time (*i.e.,* imaginary time). Therefore, the relativistic interval is

$$t^2 - \vec{x}^2 \to -\tau^2 - \vec{x}^2 < 0 \tag{125}$$

which is always space-like. Hence, with this procedure we will get the Green functions for space-like separations of its arguments. To get to time-like separations we will need to do an analytic continuation. This we will do later on. The second interpretation is that the path integral of Eq. 123 is the *partition function* of a system in Classical Statistical Mechanics in D dimensions with energy density (divided by T) equal to $\mathcal{L}_E - J\phi$. This will turn out to be a very useful connection (both ways!).

5.5.2 Finite Imaginary Time Interval

In this case we have

$$0 \leq x_0 = \tau \leq \beta = 1/T \tag{126}$$

where T will be interpreted as the temperature. Indeed, in this case the path integral is

$$Z'[0] = \text{Tr } e^{-\beta H} \tag{127}$$

and we are effectively looking at a problem of the same Quantum Field Theory but at *finite temperature* $T = 1/\beta$. The path integral is once again the partition function but of a system in Quantum Statistical Physics! The partition function thus is (I set $\hbar = 1$)

$$Z'[J] = \int \mathcal{D}\phi \; e^{-\int_0^\beta d\tau \, (\mathcal{L}_E - J\phi)} \tag{128}$$

where the field $\phi(\vec{x}, \tau)$ obeys *periodic boundary conditions* in imaginary time,

$$\phi(\vec{x}, \tau) = \phi(\vec{x}, \tau + \beta) \tag{129}$$

This boundary condition will hold for all *bosonic* theories. Theories with fermions obey instead, as we will see later on, *anti-periodic* boundary conditions.

Hence, Quantum Field Theory at finite temperature T is just Quantum Field Theory on an Euclidean space-time which is periodic (and finite) in one direction, imaginary time. In other words, we have wrapped ("compactified") Euclidean space-time into a cylinder with perimeter (circumference) $\beta = 1/T$ (in units of $\hbar = k_B = 1$).

Clearly, the Green functions in imaginary time (which we will call the Euclidean Correlation functions) are given by

$$\frac{1}{Z'[J]} \frac{\delta^N Z'[J]}{\delta J(x_1) \dots J(x_N)} \bigg|_{J=0} = \langle \phi(x_1) \dots \phi(x_N) \rangle \tag{130}$$

which are just the *correlation functions* in the equivalent problem in Statistical Mechanics. Upon analytic continuation the Euclidean Correlation Functions $\langle \phi(x_1) \dots \phi(x_N) \rangle$ and the N-point functions of the QFT are related by

$$\langle \phi(x_1) \dots \phi(x_N) \rangle \leftrightarrow (i\hbar)^N \langle 0 | T \phi(x_1) \dots \phi(x_N) | 0 \rangle \tag{131}$$

For the case of a QFT at finite temperature T, the path integral yields the correlation functions of the Heisenberg field operators in imaginary time. These correlation functions are often called the *thermal Green functions*. They are functions of the spatial positions of the fields, $\vec{x}_1, \dots, \vec{x}_N$ and of their *imaginary time coordinates*, $x_{D1}, \dots, x_{DN}$ (here $x_D \equiv \tau$). To obtain the correlation functions as a function of the *real time coordinates* $x_{01}, \dots, x_{0N}$ at *finite temperature* T it is necessary to do an analytic continuation. We will discuss how this is done later on.

5.6 Path Integrals for the Free Scalar Field

We will consider now the case of a *Free Scalar Field*. We will carry our discussion in *Euclidean Space-Time* (*i.e.,* in imaginary time), and we will do the relevant analytic continuation back to real time at the end of the calculation.

The Euclidean Lagrangian $\mathcal{L}_E$ for a free field ϕ coupled to a source J is

$$\mathcal{L}_E = \frac{1}{2} (\bigtriangledown_\mu \phi)^2 + \frac{1}{2} m^2 \phi^2 - J\phi \tag{132}$$

where we are using the notation

$$(\bigtriangledown_\mu \phi)^2 = \bigtriangledown_\mu \phi \, \bigtriangledown_\mu \, \phi \tag{133}$$

Here the index is $\mu = 1, \ldots, D$ for an Euclidean space-time of $D = d + 1$ dimensions. For the most part we will be interested in the case of $d = 3$ and Euclidean space has four dimensions. Notice the way the Euclidean space-time indices are placed in Eq. 133. This is not a misprint!

We will compute the Euclidean Path Integral (or Partition Function) $\mathcal{Z}_E[J]$ exactly. The Euclidean Path Integral for a free field has the form

$$\mathcal{Z}_E[J] = \mathcal{N} \int \mathcal{D}\phi \;\; e^{-\int d^D x \; \left[\frac{1}{2} (\bigtriangledown_\mu \phi)^2 + \frac{1}{2} m^2 \phi^2 - J\phi\right]} \tag{134}$$

In Classical Statistical Mechanics this theory is known as the Gaussian Model.

In what follows I will assume that the boundary conditions of the field ϕ (and the source J) at infinity are either vanishing or periodic, and that the source J also either vanishes at spatial infinity or is periodic. With these assumptions all terms which are total derivatives drop out identically. Therefore, upon an integration by parts and after dropping boundary terms, the Euclidean Lagrangian becomes

$$\mathcal{L}_E = \frac{1}{2} \phi \; \left[- \bigtriangledown^2 + m^2 \right] \phi - J\phi \tag{135}$$

This path integral can be calculated exactly because the action is a quadratic form of the field ϕ. It has terms which are quadratic (or, rather bilinear) in ϕ and a term linear in ϕ, the source term. By means of the following shift of the field ϕ

$$\phi(x) = \bar{\phi}(x) + \xi(x) \tag{136}$$

the Lagrangian becomes

$$\begin{aligned} \mathcal{L}_E &= \frac{1}{2} \phi \; \left[- \bigtriangledown^2 + m^2 \right] \phi - J\phi \\ &= \frac{1}{2} \bar{\phi} \; \left[- \bigtriangledown^2 + m^2 \right] \bar{\phi} - J\bar{\phi} + \frac{1}{2} \xi \; \left[- \bigtriangledown^2 + m^2 \right] \xi + \xi \; \left[- \bigtriangledown^2 + m^2 \right] \bar{\phi} - J\xi \end{aligned} \tag{137}$$

Hence, we can decouple the source $J(x)$ by requiring that the shift $\bar{\phi}$ be such that the terms linear in ξ cancel each other exactly. This requirement leads to the condition that $\bar{\phi}$ be the solution of the following partial differential equation

$$\left[- \bigtriangledown^2 + m^2 \right] \bar{\phi} = J(x) \tag{138}$$

Equivalently we can write $\bar{\phi}$ is terms of $J(x)$ through the action of the inverse of the operator $- \bigtriangledown^2 + m^2$,

$$\bar{\phi} = \frac{1}{- \bigtriangledown^2 + m^2} \; J \tag{139}$$

The solution of Eq. 138 is

$$\bar{\phi}(x) = \int d^D x' \; G_0^E(x-x') \; J(x') \tag{140}$$

where

$$G_0^E(x-x') = \langle x | \frac{1}{-\bigtriangledown^2 + m^2} | x' \rangle \tag{141}$$

is the Green function of the linear partial differential operator $-\bigtriangledown^2 + m^2$, *i.e.,* $G_0^E(x-x')$ is the solution of

$$\left[-\bigtriangledown_x^2 + m^2 \right] \; G_0^E(x-x') = \delta^D(x-x') \tag{142}$$

In terms of $G_0^E(x-x')$, the terms of the shifted action become,

$$\begin{aligned} \int d^D x \left(\frac{1}{2} \bar{\phi}(x) \; \left[-\bigtriangledown^2 + m^2 \right] \bar{\phi}(x) - J\bar{\phi}(x) \right) = & \int d^D x \left(-\frac{1}{2} \bar{\phi}(x) J(x) \right) \\ = & -\frac{1}{2} \int d^D x \; d^D x' \; J(x) \quad G_0^E(x-x') \; J(x') \end{aligned} \tag{143}$$

Therefore the path integral $Z_E[J]$, defined in Eq. 134, is given by

$$Z_E[J] = Z_E[0] \;\; e^{\displaystyle \frac{1}{2} \int d^D x \; d^D x' \; J(x) \; G_0^E(x-x') \; J(x')} \tag{144}$$

where $Z_E[0]$ is

$$Z_E[0] = \int \mathcal{D}\xi \;\; e^{\displaystyle -\frac{1}{2} \int d^D x \; \xi(x) \left[-\bigtriangledown^2 + m^2 \right] \xi(x)} \tag{145}$$

Eq. 144 shows that, after the decoupling, $Z_E[J]$ is a product of two factors: (a) a factor that is function of a bilinear form in the source J, and (b) a path integral, $Z_E[0]$, that is independent of the sources.

5.6.1 Calculation of $Z_E[0]$

The path integral $Z_E[0]$ is analogous to the fluctuation factor that we found in the path integral for a harmonic oscillator in elementary quantum mechanics. There we saw that the analogous factor could be written as a determinant of a differential operator, the kernel of the bilinear form that entered in the action. The same result holds here as well. The only difference is that the kernel is now the *partial differential* operator $\hat{A} = -\bigtriangledown^2 + m^2$ whereas in Quantum Mechanics is an ordinary differential operator. Still, the operator $\hat{A}$ has a set of eigenstates $\{\Psi_n(x)\}$ which, once the boundary conditions in space-time are specified, are both complete and orthonormal, and the associated spectrum of eigenvalues A_n is

$$\begin{aligned}
&\left[- \bigtriangledown^2 + m^2\right] \Psi_n(x) = A_n \Psi_n(x) \\
&\int d^D x \; \Psi_n(x) \; \Psi_m(x) = \delta_{n,m} \\
&\sum_n \; \Psi_n(x) \; \Psi_n(x') = \delta(x - x')
\end{aligned} \tag{146}$$

Hence, once again we can expand the field $\phi(x)$ in the complete set $\{\Psi_n(x)\}$,

$$\phi(x) = \sum_n c_n \; \Psi_n(x) \tag{147}$$

The set of field configurations is thus parametrized by the coefficients $\{c_n\}$.

The action now becomes,

$$S = \int d^D x \; \mathcal{L}_E(\phi, \partial\phi) = \frac{1}{2} \sum_n \; A_n c_n^2 \tag{148}$$

Thus, up to a normalization factor, we find that $Z_E[0]$ is given by

$$Z_E[0] = \prod_n A_n^{-1/2} \equiv \left(\text{Det}\left[- \bigtriangledown^2 + m^2\right]\right)^{-1/2} \tag{149}$$

Once again, we have reduced the calculation of $Z_E[0]$ to the computation of the determinant of a differential operator, Det $\left[- \bigtriangledown^2 + m^2\right]$.

In chapter 8 we will discuss efficient methods to compute such determinants. For the moment it will be sufficient to notice that there is a simple, but formal, way to compute this determinant. First, we notice that if we are interested in the behavior of of an infinite system at $T = 0$, the eigenstates of the operator $- \bigtriangledown^2 + m^2$ are simply suitably normalized plane waves. Let L be the linear size of the system ($L \to \infty$). Then the eigenfunctions are labeled by a D-dimensional momentum p_μ (with $\mu = 0, 1, \ldots, d$)

$$\Psi_p(x) = \frac{1}{(2\pi L)^{D/2}} e^{i \; p_\mu \; x_\mu} \tag{150}$$

with eigenvalues,

$$A_p = p^2 + m^2 \tag{151}$$

Hence the *logarithm* of determinant is

$$\begin{aligned}
\ln \text{Det}\left[- \bigtriangledown^2 + m^2\right] &= \text{Tr} \ln \left[- \bigtriangledown^2 + m^2\right] \\
&= \sum_p \; \ln(p^2 + m^2) \\
&= V \int \frac{d^D p}{(2\pi)^D} \; \ln(p^2 + m^2)
\end{aligned} \tag{152}$$

where $V = L^D$ is the volume of Euclidean space-time. Hence, (the logarithm of) $Z_E[0]$ is

$$\ln Z_E[0] = -\frac{V}{2} \int \frac{d^D p}{(2\pi)^D} \ln(p^2 + m^2) \tag{153}$$

This expression is has two singularities:

1. It diverges as $V \to \infty$. This *infrared* (IR) singularity actually is not a problem since $\ln Z_E[0]$ should be *extensive*. In other words, this is how it should behave.

2. The integral diverges at large momenta unless there is an upper bound (or *cutoff*) for the allowed momenta. This is an *ultraviolet* (UV) singularity. It has the same origin of the UV divergence of the ground state energy.

In fact $Z_E[0]$ is closely related to the ground state (vacuum) energy since

$$Z_E[0] = \lim_{\beta \to \infty} \sum_n e^{-\beta E_n} \sim e^{-\beta E_0} + \ldots \tag{154}$$

Thus,

$$E_0 = -\lim_{\beta \to \infty} \frac{1}{\beta} \ln Z_E[0] = \frac{1}{2} L^d \int \frac{d^D p}{(2\pi)^D} \ln(p^2 + m^2) \tag{155}$$

where L^d is the volume of *space*, *i. e.* $V = L^d \beta$. Notice that Eq. 155 is UV divergent. Below in this chapter we will discuss how to compute expressions of the form of Eq. 155.

5.6.2 Green Functions

A number of interesting results are found immediately by direct inspection of Eq. 144. We can easily see that, once we set $J = 0$, the Green function $G_0^E(x - x')$

$$G_0^E(x - x') = \langle x | \frac{1}{- \bigtriangledown^2 + m^2} | x' \rangle \tag{156}$$

is equal to the 2-point correlation function for this theory (at $J = 0$) ,

$$\langle \phi(x) \phi(x') \rangle = \frac{1}{Z_E[0]} \left. \frac{\delta^2 Z_E[J]}{\delta J(x) \delta J(x')} \right|_{J=0} = G_E^0(x - x') \tag{157}$$

Likewise we find that, for a free field theory, the N-point function $\langle \phi(x_1) \ldots \phi(x_N) \rangle$ is equal to

$$\begin{aligned} \langle \phi(x_1) \ldots \phi(x_N) \rangle = \frac{1}{Z_E[0]} \left. \frac{\delta^N Z_E[J]}{\delta J(x_1) \ldots \delta J(x_N)} \right|_{J=0} = \\ = \langle \phi(x_1) \phi(x_2) \rangle \ldots \langle \phi(x_{N-1}) \phi(x_N) \rangle + \text{permutations} \end{aligned} \tag{158}$$

Therefore for a free field, up to permutations of the coordinates $x_1, \ldots, x_N$, the N-point functions factorize into products of 2-point functions. Hence, N must be an positive *even* integer. This result, Eq. 158, which we derived in the context of a theory for a *free scalar* field, is actually much more general. It is known as *Wick's Theorem*. It applies to all free theories *i.e.,* theories whose Lagrangians are bilinear in the fields, it is independent of the statistics and on whether there is relativistic invariance or not. The only caveat is that, as we will see later on, for the case of fermionic theories there is a sign associated with each term of this sum. It is easy to see that, for $N = 2k$, the total number of terms in the sum is

$$(2k-1)(2k-3)\ldots\ldots = \frac{(2k)!}{2^k k!} \tag{159}$$

Each factor of a 2-point function $\langle \phi(x_1)\phi(x_2)\rangle$, *i.e.* a free propagator, and it is also called a *contraction*. It also common to use the notation

$$\langle \phi(x_1)\phi(x_2)\rangle = \phi(x_1)\phi(x_2) \tag{160}$$

to denote a contraction or propagator.

5.6.3 Calculation of the Propagator

We will now calculate the 2-point function, or propagator, $G_0^E(x-x')$ for infinite Euclidean space. This is the case of interest in QFT at $T=0$. Later on we will do the calculation of the propagator at finite temperature.

Eq. 142 tells us that $G_0^E(x-x')$ is the Green function of the operator $-\bigtriangledown^2 + m^2$. We will use Fourier transform methods and write $G_0^E(x-x')$ in the form

$$G_0^E(x-x') = \int \frac{d^D p}{(2\pi)^D}\; G_0^E(p)\; e^{i\, p_\mu (x_\mu - x'_\mu)} \tag{161}$$

which is a solution of Eq. 142 if

$$G_0^E(p) = \frac{1}{p^2+m^2} \tag{162}$$

Therefore the Green function in real (Euclidean!) space is the integral

$$G_0^E(x-x') = \int \frac{d^D p}{(2\pi)^D}\; \frac{e^{i\, p_\mu (x_\mu - x'_\mu)}}{p^2+m^2} \tag{163}$$

We will often encounter integrals of this type and for that reason we will do this one in some detail. We begin by using the identity

$$\frac{1}{A} = \frac{1}{2}\int_0^\infty d\alpha\; e^{-\frac{A}{2}\alpha} \tag{164}$$

where $A > 0$ is a positive real number. The variable α is called a Feynman-Schwinger parameter.

We now choose $A = p^2 + m^2$, and substitute this expression back in Eq. 163, which takes the form

$$G_0^E(x - x') = \frac{1}{2}\int_0^\infty d\alpha \int \frac{d^D p}{(2\pi)^D}\, e^{-\frac{\alpha}{2}(p^2 + m^2) + ip_\mu(x_\mu - x'_\mu)} \tag{165}$$

The momentum integrand is now a Gaussian, and the integral can be calculated by a shift of the integration variables p_μ, *i.e.,* by completing squares

$$\frac{\alpha}{2}(p^2 + m^2) - ip_\mu(x_\mu - x'_\mu) = \frac{1}{2}\left(\sqrt{\alpha}p_\mu - i\frac{x_\mu - x'_\mu}{\sqrt{\alpha}}\right)^2 - \frac{1}{2}\left(\frac{x_\mu - x'_\mu}{\sqrt{\alpha}}\right)^2 \tag{166}$$

and by using the Gaussian integral

$$\int \frac{d^D p}{(2\pi)^D}\, e^{-\frac{1}{2}\left(\sqrt{\alpha}p_\mu - i\frac{x_\mu - x'_\mu}{\sqrt{\alpha}}\right)^2} = (2\pi\alpha)^{-D/2} \tag{167}$$

After all of this is done, we find the formula

$$G_0^E(x - x') = \frac{1}{2(2\pi)^{D/2}} \int_0^\infty d\alpha\, \alpha^{-D/2}\, e^{-\frac{|x - x'|^2}{2\alpha} - \frac{1}{2}m^2\alpha} \tag{168}$$

Let us now define a rescaling of the variable α,

$$\alpha = \lambda t \tag{169}$$

by which

$$\frac{|x - x'|^2}{2\alpha} + \frac{1}{2}m^2\alpha = \frac{|x - x'|^2}{2\lambda t} + \frac{1}{2}m^2\lambda t \tag{170}$$

We choose

$$\lambda = \frac{|x - x'|}{m} \tag{171}$$

With this choice, the exponent becomes

$$\frac{|x - x'|^2}{2\alpha} + \frac{1}{2}m^2\alpha = \frac{m|x - x'|}{2}\left(t + \frac{1}{t}\right) \tag{172}$$

After this final change of variables, we find that the Green function is

$$G_0^E(x - x') = \frac{1}{(2\pi)^{D/2}}\left(\frac{m}{|x - x'|}\right)^{\frac{D}{2} - 1} K_{\frac{D}{2}-1}(m|x - x'|) \tag{173}$$

where $K_\nu(z)$ is the Bessel function (of imaginary argument, see *e.g.* Gradshteyn and Ryzhik) which has the integral representation

$$K_\nu(z) = \frac{1}{2}\int_0^\infty dt\, t^{\nu - 1}\, e^{-\frac{z}{2}\left(t + \frac{1}{t}\right)} \tag{174}$$

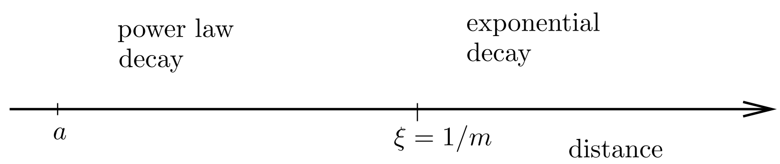


Figure 5: Behaviors of the Euclidean Green Function.

with $\nu = \frac{D}{2} - 1$, and $z = m|x - x'|$.

There are two interesting regimes: (a) long distances, $m|x - x'| \gg 1$, and (b) short distances, $m|x - x'| \ll 1$.

1. *Long Distance Behavior*:
   In this regime, $z = m|x - x'| \gg 1$, a saddle-point calculation shows that the Bessel Function $K_\nu(z)$ has the asymptotic behavior,

$$K_\nu(z) \approx \sqrt{\frac{\pi}{2z}} e^{-z} \left[1 + O(1/z)\right] \tag{175}$$

   Thus, in this regime the Euclidean Green function behaves like

$$G_0^E(x - x') \approx \frac{\sqrt{\pi/2}\, m^{D-2}\, e^{-m|x-x'|}}{(2\pi)^{D/2}\,(m|x-x'|)^{\frac{D-1}{2}}} \left[1 + O\left(\frac{1}{m|x-x'|}\right)\right] \tag{176}$$

   Therefore, at long distances, the Euclidean (or imaginary time) Green function has an exponential decay with distance (and imaginary time). The length scale for this decay is $1/m$, which is natural since it is the only quantity with units of length in the theory. In real time, and in conventional units, this length scale is just the Compton wavelength, $\hbar/mc$. In Statistical Physics this length scale is known as the *correlation length* ξ.

2. *Short Distance Behavior*:
   In this regime we must use the behavior of the Bessel function for small values of the argument,

$$K_\nu(z) \approx \frac{\Gamma(\nu)}{2\left(\frac{z}{2}\right)^\nu} + O(1/z^{\nu-2}) \tag{177}$$

   The Green function now behaves instead like,

$$G_0^E(x - x') \approx \frac{\Gamma(\frac{D}{2} - 1)}{4\pi^{D/2}|x - x'|^{D-2}} + \dots \tag{178}$$

   where $\dots$ are terms that vanish as $m|x - x'| \to 0$. Notice that the leading term is *independent of the mass* m. This is the behavior of the *massless* theory.

5.6.4 Behavior of the Green function in Minkowski space

We must now address the issue of the behavior of the Green function in *real time*. This means that now we must do the analytic continuation back to real time x_0. In what follows we will set $D = 4$.

Let us recall that in going from Minkowski to Euclidean space we continued $x_0 \to -ix_4$. There is also factor of i difference in the definition of the Green function. Thus, the Green function in Minkowski space $G_0(x-x')$ is the expression that results from

$$G_0(x-x') = i\, G_0^E(x-x')\big|_{x_4 \to ix_0} \tag{179}$$

The relativistic interval s is given by

$$s^2 = (t-t')^2 - (\vec{x} - \vec{x}\,')^2 \tag{180}$$

The Euclidean interval (length) $|x-x'|$, and the relativistic interval s are related by

$$|x-x'| = \sqrt{(x-x')^2} \to \sqrt{-s^2} \tag{181}$$

Therefore, in $D = 4$ space-time dimensions, the Minkowski space propagator is

$$G_0(x-x') = \frac{i}{4\pi^2} \frac{m}{\sqrt{-s^2}}\, K_1(m\sqrt{-s^2}) \tag{182}$$

we will need the asymptotic behavior of the Bessel function $K_1(z)$,

$$\begin{aligned} K_1(z) = & \quad \sqrt{\frac{\pi}{2z}} e^{-z} \left[1 + \frac{3}{8z} + \ldots\right] & , \text{ for } z \gg 1 \\ K_1(z) = & \quad \frac{1}{z} + \frac{z}{2}\left(\ln z + C - \frac{1}{2}\right) + \ldots & , \text{ for } z \ll 1 \end{aligned} \tag{183}$$

where $C = 0.577215\ldots$ is the Euler constant. Let us examine the behavior of Eq. 182 in the regimes: (a) space-like, $s^2 < 0$, and (b) time-like, $s^2 > 0$, intervals.

1. $(x-x')^2 = s^2 < 0$
   This is the space-like domain. By inspecting Eq. 182 we see that for space-like separations, the factor $\sqrt{-s^2}$ is a positive real number. Consequently the argument of the Bessel function is real (and positive), and the Green function is pure imaginary. In particular we see that, for $s^2 < 0$ the Minkowski Green function is essentially the Euclidean Green function,

$$G_0(x-x') = iG_0^E(x-x') \qquad , \text{ for } s^2 < 0 \tag{184}$$

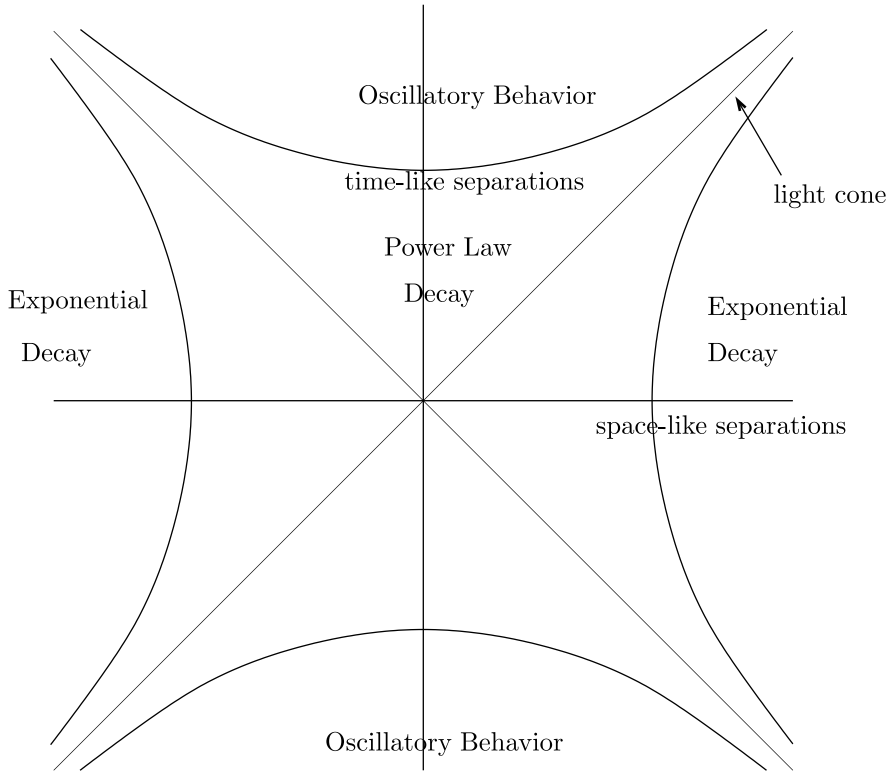


Figure 6: Behaviors of the Green Function in Minkowski space-time.

Hence, for $s^2 < 0$ we have the behaviors,

$$G_0(x-x') \approx i\frac{\sqrt{\pi/2}}{4\pi^2}\frac{m^2}{\left(m\sqrt{-s^2}\right)^{3/2}}e^{-m\sqrt{-s^2}} \qquad , \text{ for } m\sqrt{-s^2} \gg 1$$
$$G_0(x-x') \approx \frac{i}{4\pi^2(-s^2)} \qquad , \text{ for } m\sqrt{-s^2} \ll 1 \tag{185}$$

2. $(x-x')^2 = s^2 > 0$
This is the time-like domain. The analytic continuation yields

$$G_0(x-x') = \frac{m}{4\pi^2\sqrt{s^2}}K_1(im\sqrt{s^2}) \tag{186}$$

For pure imaginary arguments, the Bessel function $K_1(iz)$ is the analytic continuation of the Hankel function, $K_1(iz) = -\frac{\pi}{2}H_1^{(1)}(-z)$. This function is oscillatory for large values of its argument. Indeed, we now get the behaviors

$$
\begin{aligned}
G_0(x-x') &\approx \frac{\sqrt{\pi/2}}{4\pi^2}\frac{m^2}{\left(m\sqrt{s^2}\right)^{3/2}}e^{im\sqrt{s^2}} \qquad &, \text{ for } m\sqrt{s^2}\gg 1\\
G_0(x-x') &\approx \frac{1}{4\pi^2 s^2} &, \text{ for } m\sqrt{s^2}\ll 1
\end{aligned}
\tag{187}
$$

Notice that, up to a factor of i, the short distance behavior is the same for both time-like and space like separations. The main difference is that at large time-like separations we get an oscillatory behavior instead of an exponential decay. The length scale of the oscillations is, once again, set by the only scale in the theory, the Compton wavelength.

5.6.5 Exponential decays and mass gaps

The exponential decay at long space-like separations (and the oscillatory behavior at long time-like separations) is not a peculiarity of the free field theory. It is a general consequence of the existence of a *mass gap* in the spectrum. We can see that by considering the 2-point function of a *generic* theory, for simplicity in imaginary time. The 2-point function is

$$
G^{(2)}(\vec{x}-\vec{x}\,',\tau-\tau') = \langle 0|T\hat{\phi}(\vec{x},\tau)\hat{\phi}(\vec{x}\,',\tau')|0\rangle \tag{188}
$$

where T is the imaginary time-ordering operator.

The Heisenberg representation of the operator $\hat{\phi}$ in imaginary time is ($\hbar=1$)

$$
\hat{\phi}(\vec{x},\tau) = e^{H\tau}\;\hat{\phi}(\vec{x},0)\;e^{-H\tau} \tag{189}
$$

Hence, we can write the 2-point function as

$$
\begin{aligned}
& G^{(2)}(\vec{x}-\vec{x}\,',\tau-\tau') = \\
= \quad & \theta(\tau-\tau')\langle 0|e^{H\tau}\;\hat{\phi}(\vec{x},0)\;e^{-H(\tau-\tau')}\;\hat{\phi}(\vec{x}\,',0)\;e^{-H\tau'}|0\rangle \\
+ \quad & \theta(\tau'-\tau)\langle 0|e^{H\tau'}\;\hat{\phi}(\vec{x}\,',0)\;e^{-H(\tau'-\tau)}\;\hat{\phi}(\vec{x},0)\;e^{-H\tau}|0\rangle \\
= \quad & \theta(\tau-\tau')\;e^{E_0(\tau-\tau')}\;\langle 0|\hat{\phi}(\vec{x},0)\;e^{-H(\tau-\tau')}\;\hat{\phi}(\vec{x}\,',0)|0\rangle \\
+ \quad & \theta(\tau'-\tau)\;e^{E_0(\tau'-\tau)}\;\langle 0|\hat{\phi}(\vec{x}\,',0)\;e^{-H(\tau'-\tau)}\;\hat{\phi}(\vec{x},0)|0\rangle
\end{aligned}
\tag{190}
$$

We now insert a complete set of eigenstates $\{|n\rangle\}$ of the Hamiltonian $\hat{H}$, with eigenvalues $\{E_n\}$. The 2-point function now reads,

$$
\begin{aligned}
& G^{(2)}(\vec{x}-\vec{x}\,', \tau-\tau') = \\
&= \theta(\tau-\tau') \sum_n \langle 0|\hat{\phi}(\vec{x},0)|n\rangle \, \langle n|\hat{\phi}(\vec{x}\,',0)|0\rangle \; e^{-(E_n - E_0)(\tau-\tau')} \\
&+ \theta(\tau'-\tau) \sum_n \langle 0|\hat{\phi}(\vec{x}\,',0)|n\rangle \, \langle n|\hat{\phi}(\vec{x},0)|0\rangle \; e^{-(E_n - E_0)(\tau'-\tau)}
\end{aligned}
\tag{191}
$$

Since

$$
\hat{\phi}(\vec{x},0) = e^{i\hat{\vec{P}}\cdot\vec{x}}\hat{\phi}(0,0)e^{-i\hat{\vec{P}}\cdot\vec{x}} \tag{192}
$$

and that

$$
\hat{\vec{P}}|0\rangle = 0, \qquad \hat{\vec{P}}|n\rangle = \vec{P}_n, \tag{193}
$$

where $\vec{P}_n$ is the linear momentum of state $|n\rangle$, we can write

$$
\langle 0|\hat{\phi}(\vec{x},0)|n\rangle \, \langle n|\hat{\phi}(\vec{x}\,',0)|0\rangle = |\langle 0|\hat{\phi}(0,0)|n\rangle|^2 \; e^{-i\vec{P}_n\cdot(\vec{x}-\vec{x}\,')} \tag{194}
$$

using the above expressions we can write the expressions in Eq. 191 in the form

$$
\begin{aligned}
& G^{(2)}(\vec{x}-\vec{x}\,', \tau-\tau') = \sum_n |\langle 0|\hat{\phi}(0,0)|n\rangle|^2 \\
& \times \Big[\theta(\tau-\tau')e^{-i\vec{P}_n\cdot(\vec{x}-\vec{x}\,')}e^{-(E_n - E_0)(\tau-\tau')} \\
& +\theta(\tau'-\tau)e^{-i\vec{P}_n\cdot(\vec{x}\,'-\vec{x})}e^{-(E_n - E_0)(\tau'-\tau)}\Big]
\end{aligned}
\tag{195}
$$

Thus, at equal positions, $\vec{x}=\vec{x}\,'$, we obtain the simpler expression in the imaginary time interval $\tau-\tau'$

$$
G^{(2)}(0,\tau-\tau') = \sum_n |\langle 0|\hat{\phi}(\vec{x},0)|n\rangle|^2 \times e^{-(E_n - E_0)|\tau-\tau'|} \tag{196}
$$

In the limit of large imaginary time separation, $|\tau-\tau'|\to\infty$, there is always a largest non-vanishing term in the sums. This is the term for the state $|n_0\rangle$ that mixes with the vacuum state $|0\rangle$ through the field operator $\hat{\phi}$, and with the *lowest* excitation energy or *mass gap* $E_{n_0}-E_0$. Hence, for $|\tau-\tau'|\to\infty$, the 2-point function decays exponentially like,

$$
G^{(2)}(0,\tau-\tau') \simeq |\langle 0|\hat{\phi}(\vec{x},0)|n_0\rangle|^2 \times e^{-(E_{n_0} - E_0)|\tau-\tau'|} \tag{197}
$$

Therefore, if the spectrum has a gap, the correlation functions (or Green functions) decay exponentially in imaginary time. In real time we get an oscillatory behavior. This is a very general result. Finally, notice that Lorentz invariance in Minkowski space-time (real time) implies rotational (Euclidean) invariance in imaginary time. Hence, exponential decay in imaginary times, at equal positions, must imply (in general) exponential decay in real space at equal imaginary times (an laos in real time since the time difference in this case vanishes). Thus, in a Lorentz invariant system the propagator at space-like separations is always equal to the propagator in imaginary time.