Chapter 4

Gaussian functional integrals

A very important class of Feynman propagators results from Lagrangians which are quadratic forms of $x(t)$ and $\dot{x}(t)$:

$$L(\dot{x},x,t) = a(t)\,\dot{x}^2(t) + b(t)\,\dot{x}x + c(t)\,x^2 + d(t)\dot{x} + e(t)\,x + f(t)\,. \qquad (4.1)$$

In this case the propagator

$$K(x_b,x_a,t_b-t_a) = \int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt L(\dot{x},x,t)}\ ,$$

is evaluated as follows. We decompose the quantal trajectory into the classical trajectory, $\bar{x}(t)$,

$$\delta S[x(t)] = 0 \qquad \text{gives} \qquad \bar{x}(t)\ , \qquad (4.2)$$

and a fluctuation, $y(t)$, around it

$$x(t) = \bar{x}(t) + y(t)\,, \qquad y(t_b) = y(t_a) = 0\,. \qquad (4.3)$$

The action $S[x(t)]$ is stationary around $\bar{x}(t)$, hence terms linear in $y(t)$ vanish. Thus

$$S[\bar{x}(t)+y(t)] = S[\bar{x}(t)] + \tfrac{1}{2}\delta^2 S[y(t)] \qquad (4.4)$$

where

$$\tfrac{1}{2}\delta^2 S[y(t)] = \int_{t_a}^{t_b} dt \Big(a(t)\dot{y}^2 + b(t)\dot{y}y + c(t)y^2 \Big)\,. \qquad (4.5)$$

Since $\bar{x}(t)$ is fixed, the integration over paths reduces to integrating over all $y(t)$'s which vanish at the ends, thus $\mathcal{D}x(t) = \mathcal{D}y(t)$ and

$$K(x_b,x_a,t_b-t_a) = F(t_b-t_a)\, e^{\frac{i}{\hbar}S[\bar{x}(t)]}\,, \qquad (4.6)$$

with

$$F(t_b-t_a) = \int [\mathcal{D}y(t)]\, e^{\frac{i}{\hbar}\frac{1}{2}\delta^2 S[y(t)]} \qquad (4.7)$$

where $F(t_b-t_a)$ does not depend on the spatial positions because they are always equal zero.

Equation (4.6) tells us that when L is a quadratic form of $\dot{x}(t)$ and $x(t)$ the dependence of K on x_b and x_a is completely determined by the classical trajectory $\bar{x}(t)$ (more specifically: by the value of the functional of action, $S[\bar{x}(t)]$, calculated at $\bar{x}(t)$). One may interpret the prefactor $F(t_b - t_a)$ as the contribution of quantal fluctuations around the classical trajectory. Note, however, that although $\exp\{iS[\bar{x}(t)]/\hbar\}$ is uniquely determined by the classical trajectory, it is, nevertheless, a quantal object.

We are going to discuss now a few important examples of Gaussian propagators.

4.1 A free particle

We already have expression for it, eq.(1.39)

$$K_0(b,a) = \int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{1}{2}m\dot{x}^2\, dt} = \sqrt{\frac{m}{2i\pi\hbar(t_b - t_a)}}\, e^{i\frac{1}{2}m\frac{(x_b - x_a)^2}{\hbar(t_b - t_a)}} .$$

$S[\bar{x}(t)]$ is trivially simple to evaluate, however the prefactor is not that obvious. In fact this situation is typical: the prefactor is, as a rule, the main problem.

4.2 The harmonic oscillator

Now we have to evaluate

$$K(x_b, x_a, t_b - t_a) = \int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{1}{2}m(\dot{x}^2 - \omega^2 x^2)\, dt} = F(T)\, e^{\frac{i}{\hbar}S[\bar{x}(t)]} \tag{4.8}$$

where $T = t_b - t_a$, and

$$\bar{x}(t) = \frac{1}{\sin\omega T}\,\left[x_b \sin\omega(t - t_a) + x_a \sin\omega(t_b - t)\right] \tag{4.9}$$

$\bar{x}(t)$ satisfies the correct boundary conditions

$$\bar{x}(t_a) = x_a\,, \qquad\qquad \bar{x}(t_b) = x_b\,. \tag{4.10}$$

With the help of (4.9) we get

$$S[\bar{x}(t)] = \int_{t_a}^{t_b} \tfrac{1}{2}m(\dot{\bar{x}}^2 - \omega^2\bar{x}^2)\, dt = \frac{m\omega}{2\sin\omega T}\,\left[(x_b^2 + x_a^2)\cos\omega T - 2x_b x_a\right], \tag{4.11}$$

and it remains to evaluate the prefactor

$$F(t_b - t_a) = \int [\mathcal{D}y(t)]\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{1}{2}m(\dot{y}^2 - \omega^2 y^2)\, dt}\,. \tag{4.12}$$

Note that the system does not distinguish any specific time, hence the amplitude may depend only on the difference $T = t_b - t_a$.

One of the methods of calculating (4.12) is to change the variables and reduce the integrals to simple Gaussians. One does it through a Fourier transformation

$$y(t) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi t}{T}\,, \qquad n > 0\,, \tag{4.13}$$

and negative n's can be absorbed in the definition of a_n's. This representation of $y(t)$ satisfies the boundary conditions, $y(0) = y(T) = 0$. Now we have (note that functions $\sin \frac{n\pi t}{T}$ (and $\cos \frac{n\pi t}{T}$) form a complete set of orthogonal functions over the time interval $0 \le t \le T$):

$$\int_0^T \frac{1}{2} m(\dot{y}^2 - \omega^2 y^2)\, dt \;=\; \frac{1}{2} m \frac{T}{2} \sum_n \left(\left(\frac{n\pi}{T}\right)^2 - \omega^2 \right) a_n^2\,. \tag{4.14}$$

Changing integrations over paths from integrations over $y(t)$'s to integrations over a_n's introduces into the right hand side of (4.12) all kinds of factors, *but we do not need to calculate them.* This is so because we know the normalization of F in the limit $\omega \to 0$ which just the free particle prefactor

$$F_{\omega=0}(T) \;=\; \sqrt{\frac{m}{2\pi i\hbar T}}\,. \tag{4.15}$$

So, as long as we do not skip any factors containig ω we do not bother about normalizations and get (we start with a finite number of modes)

$$F(T) = C' \prod_{n=1}^{N} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}\frac{m}{2}\frac{T}{2}[\frac{n^2\pi^2}{T^2} - \omega^2]\, a_n^2} = C \prod_{n=1}^{N} \left(1 - \frac{\omega^2 T^2}{n^2\pi^2} \right)^{-\frac{1}{2}}. \tag{4.16}$$

But (compare ref. [4.1])

$$\lim_{N\to\infty} \prod_{n=1}^{N} \left(1 - \frac{\omega^2 T^2}{n^2\pi^2} \right)^{-\frac{1}{2}} = \left(\frac{\sin \omega T}{\omega T} \right)^{-\frac{1}{2}}\,, \tag{4.17}$$

therefore, from (4.15), the harmonic oscillator prefactor is

$$F(T) \;=\; \left(\frac{m\omega}{2\pi i\hbar \sin \omega T} \right)^{\frac{1}{2}}\,, \tag{4.18}$$

and the complete expression for the propagator is

$$K(x_b, x_a, T) \;=\; \left(\frac{m\omega}{2\pi i\hbar \sin \omega T} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\frac{m\omega}{2\sin\omega T}[(x_b^2 + x_a^2)\cos\omega T - 2x_b x_a]}\,. \tag{4.19}$$

4.3 Forced harmonic oscillator

Now the Lagrangian is

$$L(\dot{x}(t), x(t), t) = \tfrac{1}{2} m\dot{x}^2 - \tfrac{1}{2} m\omega^2 x^2 + f(t)\, x \tag{4.20}$$

where $f(t)$ is a given, time dependent, external force applied to the oscillator. From the discussion presented above it is clear that the prefactor stays the same (given by (4.18)) but we have to calculate $S[\bar{x}(t)]$.

Here are a few pointers on how to do it. We solve the classical equations of motion

$$\ddot{\bar{x}} + \omega^2 \bar{x} = \frac{f(t)}{m} = j(t) \tag{4.21}$$

with the help of a Green function. The solution is in the form:

$$\bar{x}(t) = x_0(t) + x_f(t) \quad \text{where} \quad x_f(t) = \int_{t_a}^{t_b} G(t,s)\, j(s) ds\,, \tag{4.22}$$

and $x_0(t)$ is the solution of the homogeneous equation

$$\ddot{x}_0 + \omega^2 x_0 = 0 \tag{4.23}$$

satisfying the boundary conditions: $x_0(t_a) = x_a$, $x_0(t_b) = x_b$, whereas $G(t,s)$ is the solution of the inhomogeneous equation

$$\frac{d^2}{dt^2} G(t,s) + \omega^2 G(t,s) = \delta(t-s) \tag{4.24}$$

with the boundary conditions $G(t_b, s) = G(t_a, s) = 0$. These conditions guarantie that at $t = t_a$ and $t = t_b$, $x_f(t)$ does not change the boundary values of $\bar{x}(t)$ set by $x_0(t)$.

The standard method of finding $G(t,s)$ is to construct it from two independent solutions of the homogeneous equation. Let $u(t)$ and $v(t)$ be such solutions that $u(t_a) = 0$ and $v(t_b) = 0$. For $t > s$ let $G(t,s)$ as a function of t be proportional to $u(t)$, and for $t < s$ to $v(t)$. Then $G(t,s)$ satisfies (4.24) everywhere except $t = s$. To get a δ function at $t = s$ we have to fix dependences on s and the normalization. Indeed, the following construction satisfies all conditions stated above:

$$G(t,s) = -\frac{1}{\omega \sin \omega T}\; [\theta(s-t)\, v(s) u(t) + \theta(t-s)\, u(s) v(t)] \tag{4.25}$$

with $u(t) = \sin \omega(t - t_a)$ and $v(t) = \sin \omega(t_b - t)$.

To obtain $S[\bar{x}(t)]$ it is convenient, before employing $\bar{x}(t)$ calculated above, to integrate by parts the term of S containing $\bar{x}$, and then use (4.21). Thus we obtain the following convenient form of the classical action:

$$S[\bar{x}(t)] = \tfrac{1}{2} m [x_b \dot{\bar{x}}(t_b) - x_a \dot{\bar{x}}(t_a)] + \tfrac{1}{2} \int_{t_a}^{t_b} dt f(t) \bar{x}(t)\,. \tag{4.26}$$

Inserting $\bar{x}(t)$ obtained from (4.22) we find

$$\begin{aligned} S[\bar{x}(t)] &= \frac{m\omega}{2\sin\omega T}\Bigg\{(x_a^2+x_b^2)\cos\omega T - 2x_a x_b \\ &+ \frac{2x_b}{m\omega}\int_{t_a}^{t_b} dt f(t)\sin\omega(t-t_a) + \frac{2x_a}{m\omega}\int_{t_a}^{t_b} dt f(t)\sin\omega(t_b-t) \\ &- \frac{2}{m^2\omega^2}\int_{t_a}^{t_b} dt \int_{t_a}^{t} ds f(t) f(s)\sin\omega(t_b-t)\sin\omega(s-t_a)\Bigg\}. \end{aligned} \tag{4.27}$$

4.4 The van Vleck formula for the prefactor

There is a formula which gives the prefactor through differentiation of the action calculated for a classical trajectory $\bar{x}(t)$:

$$F(t_b-t_a) = \left(-\frac{1}{2\pi i\hbar}\frac{\partial^2 S(x_b,x_a,t_b-t_a)}{\partial x_b \partial x_a}\right)^{\frac{1}{2}}. \tag{4.28}$$

Note that the Gaussian actions are always quadratic functions of x_a and x_b, thus F from (4.28) depends only on $T = t_b - t_a$, as it should be. Indeed, applying (4.28) to (4.27) we obtain the correct prefactor which we have calculated for the harmonic oscillator.

The justification of the van Vleck formula (4.28) can be done in many ways. Let us start with some classical physics arguments, which give an intuitive explanation of the formula. From (4.6) we see that the probability density of transition from (x_a, t_a) to (x_b, t_b) is

$$|K(x_b,x_a,t_b-t_a)|^2 = |F(t_b-t_a)|^2 = P(t_b-t_a)\,,. \tag{4.29}$$

The best one can do through classical description of the evolution of our system is to calculate $P(t_b - t_a)$, and obtain $F = \sqrt{P}\,e^{i\phi}$ with an undetermined phase factor.

In order to determine P we look at the fan of classical trajectories around $\bar{x}(t)$ which leads from (x_a, t_a) to (x_b, t_b). This fan of trajectories is given by $\bar{x}(t)+\delta x(t)$ where $\delta x(t_a) = 0$, but we shall vary the initial velocities (momenta)

$$m\,\delta\dot{x}(t_a) = \delta p_a\,. \tag{4.30}$$

In the lowest order, $\delta x(t)$ satisfies the equation

$$m\,\frac{d^2\delta x}{dt^2} = -\frac{\partial^2 V}{\partial x^2}\bigg|_{\bar{x}(t)}\delta x\,. \tag{4.31}$$

All trajectories start from x_a but with different momenta $p_a + \delta p_a$. The spread of δp_a's determines the spread of final positions δx_b at t_b. We relate δx_b with δp_a with the help of relations between the derivatives of the action and momenta. In our case we need

$$\frac{\partial S(x_b,x_a,t_b-t_a)}{\partial x_a} = -p_a\,. \tag{4.32}$$

Thus, as long as the spread is small,

$$-\delta p_a = \frac{\partial^2 S}{\partial x_a \partial x_b}\delta x_b \,, \tag{4.33}$$

and

$$\mathcal{N}^{-1} = -\frac{\partial^2 S}{\partial x_a \partial x_b} \,, \tag{4.34}$$

(which becomes a matrix for more than one dimensions) give us the spread of the fan of trajectories around $\bar{x}(t)$

$$\delta x_b \, = \mathcal{N}\, \delta p_a \,. \tag{4.35}$$

When the classical motion is reversible in time, $\mathcal{N}^{-1}$ is a symmetric matrix in more than one dimensions, hence its eigenvalues are real (but depend on t). It may happen that $\mathcal{N}^{-1}$ is singular at a certain time. For instance, for the harmonic oscillator

$$\mathcal{N}_{\rm osc}^{-1} \; = \; \frac{m\omega}{\sin\omega(t_b - t_a)} \,, \tag{4.36}$$

hence, for $t_b - t_a = n\pi/\omega$ where $n = 0, 1, 2, ...$, we have $\mathcal{N} = 0$ and $\delta x_b = 0$. So, for these lapses of time, different p_a's give the same position as $\bar{x}$. Note the consequence of this fact: there are *infinitely many trajectories going from* (x_a, t_a) *to* (x_b, t_b).

$\mathcal{N}$ gives us a time-dependent measure of the size of the fan of trajectories emerging from the initial position x_a. The smaller is $\mathcal{N}$ the denser is the fan of trajectories surrounding $\bar{x}$. Thus $dx_b \mathcal{N}^{-1} dx_a$ – if properly normalized – could measure the probability of going from the neighborhood of x_a to the neighborhood of x_b . Since its dimension is that of an action, it is tempting to convert it into a quantal expression dividing it by $2\pi\hbar = h$. Then we get

$$P(t_b - t_a) \; = \; \frac{1}{2\pi\hbar}\frac{\partial^2 S(x_b, x_a, t_b - t_a)}{\partial x_a \partial x_b} \; = \; |F(t_b - t_a)|^2 \,. \tag{4.37}$$

This is indeed consistent with (4.28).

Before closing this section let us point out that the prefactor $F(T)$, eq.(4.12), can also be calculated directly from its original form by doing integration over N variables $y_1, y_2, ..., y_N$ and then taking $N \to \infty$. So, we have to calculate

$$F(t_b, t_a) = \lim_{N\to\infty}\int dy_1 dy_2 ... \, dy_N \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N+1}{2}} e^{\frac{i}{\hbar}\sum_{j=0}^{N}\frac{1}{2}m\,[\frac{(y_{j+1}-y_j)^2}{\epsilon} - \epsilon\omega^2 y_j^2]} \,. \tag{4.38}$$

First, we write the exponent of (4.38) in matrix notation:

$$-\frac{m}{2i\hbar\epsilon}\sum_{j=0}^{N}\left[(y_{j+1} - y_j)^2 - \epsilon^2\omega^2 y_j^2\right] = -\mathcal{Y}^T \Lambda \mathcal{Y} \tag{4.39}$$

where

$$\Lambda_{i,k} = \frac{m}{2i\hbar\epsilon}\Big([2\delta_{i,k} - \delta_{i,k-1} - \delta_{i,k+1}] - \epsilon^2\omega^2\delta_{i,k}\Big) = \frac{m}{2i\hbar\epsilon}\sigma_{i,k} \tag{4.40}$$

and

$$\mathcal{Y}^T = (y_1, y_2, ...y_N)\,. \tag{4.41}$$

Thus $\mathcal{Y}$ is a column matrix. To see that (4.39) is correct we must remember that

$$y_0 = y_{N+1} = y(t_a) = y(t_b) = 0\,. \tag{4.42}$$

Indeed,

$$\sum_{j=0}^{N} y_j y_{j+1} = \sum_{j=0}^{N} y_j y_{j-1} \qquad \text{and} \qquad 2\sum_{j=0}^{N} y_j^2 = \sum_{j=0}^{N} y_j^2 + \sum_{j=0}^{N} y_{j+1}^2\,.$$

Now, we can write

$$F(t_b, t_a) = \lim_{N\to\infty} \int d^N\mathcal{Y} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N+1}{2}} e^{-\mathcal{Y}^T\Lambda\,\mathcal{Y}}\,. \tag{4.43}$$

Since σ of (4.40) is a real and symmetric matrix we can diagonalise it with the help of an orthogonal matrix $\mathcal{O}$. Transforming also $\mathcal{Y}$ into $\nu = \mathcal{O}\mathcal{Y}$, and noticing that the Jacobian of this transformation is 1 (because $|\det\mathcal{O}| = 1$) we get

$$\int d^N\mathcal{Y}\, e^{-\mathcal{Y}^T\Lambda\mathcal{Y}} = \prod_{l=1}^{N} \int_{-\infty}^{+\infty} d\nu_l\, e^{-\nu_l^2\Lambda_l} = \prod_{l=1}^{N} \sqrt{\frac{\pi}{\Lambda_l}} = \frac{\pi^{N/2}}{\sqrt{\det\Lambda}} \tag{4.44}$$

where Λ_l ‘s are the eigevalues of Λ.

Since $\det\Lambda = (m/2i\hbar\epsilon)^N \det\sigma$, it is convenient to introduce the following object

$$\tilde{\mathcal{N}}_N = \epsilon \left(\frac{2i\hbar\epsilon}{m}\right)^N \det\Lambda = \epsilon\det\sigma\,. \tag{4.45}$$

Let us write now

$$F(t_b, t_a) \;=\; \lim_{N\to\infty} \sqrt{\frac{m}{2\pi i\hbar}\frac{1}{\tilde{\mathcal{N}}_N}} \;=\; \sqrt{\frac{m}{2\pi i\hbar}\frac{1}{\tilde{\mathcal{N}}}} \tag{4.46}$$

where

$$\tilde{\mathcal{N}} \;=\; \lim_{N\to\infty} \tilde{\mathcal{N}}_N \;=\; \lim_{N\to\infty} \left\{ \epsilon \left(\frac{2\pi i\hbar\epsilon}{m}\right)^N \det\Lambda \right\}\,. \tag{4.47}$$

In order to calculate $\tilde{\mathcal{N}}$ we define $\tilde{\mathcal{N}}_j$ as obtained from the first j rows and columns of Λ (or σ). It is not too difficult to find following recurrence relation for $\tilde{\mathcal{N}}_j$

$$\tilde{\mathcal{N}}_{j+1} = (2 - \epsilon^2\omega^2)\tilde{\mathcal{N}}_j - \tilde{\mathcal{N}}_{j-1}\,, \qquad j = 1, 2, ..., N \tag{4.48}$$

with the following initial values

$$\tilde{\mathcal{N}}_0 = \epsilon \quad \text{and} \quad \tilde{\mathcal{N}}_1 = \epsilon(2 - \epsilon^2\omega^2)\,. \tag{4.49}$$

eq.(4.48) can also be written as

$$\frac{1}{\epsilon^2}(\tilde{\mathcal{N}}_{j+1} - 2\tilde{\mathcal{N}}_j + \tilde{\mathcal{N}}_{j-1}) = -\omega^2\tilde{\mathcal{N}}_j\,. \tag{4.50}$$

In the continuum limit, $t = t_a + T$ with $T = j\epsilon$, where $j \to \infty$ and $\epsilon \to 0$ keeping T fixed, we get from (4.50)

$$\frac{d^2\tilde{\mathcal{N}}}{dt^2} = -\,\omega^2\tilde{\mathcal{N}}\,. \tag{4.51}$$

The initial conditions we obtain from (4.49):

$$\begin{aligned} \tilde{\mathcal{N}}(t=0) &= \tilde{\mathcal{N}}_0 \;=\; 0\,, \\ \frac{d\tilde{\mathcal{N}}}{dt}(t=0) &= \frac{\tilde{\mathcal{N}}_1 - \tilde{\mathcal{N}}_0}{\epsilon} \;=\; \frac{\epsilon(2-\epsilon^2\omega^2)-\epsilon}{\epsilon} \;=\; 1\;. \end{aligned} \tag{4.52}$$

So, $\tilde{\mathcal{N}}(t_b) = \tilde{\mathcal{N}}(t_b, t_a)$ is the solution of (4.51) with the initial conditions

$$\tilde{\mathcal{N}}(0) = 0\,, \qquad \frac{\partial\tilde{\mathcal{N}}}{\partial t}(t=0) = 1\,, \tag{4.53}$$

which is

$$\tilde{\mathcal{N}}(t_b, t_a) = \frac{\sin\omega(t_b - t_a)}{\omega} = \frac{\sin\omega T}{\omega}\,. \tag{4.54}$$

Comparing with the previously defined $\mathcal{N}$ we find $\tilde{\mathcal{N}} = m\mathcal{N}$.

Note that $\mathcal{N}$ which measures the spread in space of classical trajectories is, on the other hand, given by the product of the eigenvalues Λ_l.