Chapter 13

Constrained systems

In this section the implementation of constraints within the path integral formalism is discussed. The study of constraints is quantum mechanics is subtle and significant, since constraints are closely related to symmetries. All gauge theories are systems with constraints and conversely: all systems with first class constraints are gauge theories.

We shall see that, with some important adjustments to the measure, the path integral quantization for constrained system is very similar to the previously discussed path integral for unconstrained systems.

In a classical mechanical system whose phase space consists of $2n$ degrees of freedom $\{q^1, \ldots, q^n, p_1, \ldots, p_n\}$, a constraint consists of some relation between the coordinates. To illustrate what may happen in such cases, we first study a simple mechanical system for two point-'particles', confined to a line and governed by a Hamiltonian

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(q^1 - q^2). \tag{13.1}$$

Since the interaction depends only on the distance of the two particles the total momentum is conserved

$$\frac{d}{dt}P = \frac{i}{\hbar}[H, P] = 0. \tag{13.2}$$

After a canonical transformation to the center of mass Q and the relative coordinate q,

$$\begin{aligned} Q &= \frac{m_1}{M}q^1 + \frac{m_2}{M}q^2 \quad , \quad P = p_1 + p_2 \\ q &= q^1 - q^2 \qquad\qquad\quad , \quad p = \frac{m_2}{M}p_1 - \frac{m_1}{M}p_2 \end{aligned} \tag{13.3}$$

the inverse transformation of which reads

$$\begin{aligned} q^1 &= Q + \frac{m_2}{M}q \quad , \quad p_1 = \frac{m_1}{M}P + p, \\ q^2 &= Q - \frac{m_1}{M}q \quad , \quad p_2 = \frac{m_2}{M}P - p, \end{aligned} \tag{13.4}$$

where $M = m_1 + m_2$ is the total mass of the system, the Hamiltonian takes the form

$$H = \frac{P^2}{2M} + \frac{p^2}{2\mu} + V(q) = \frac{P^2}{2M} + H_{CM}(p, q). \tag{13.5}$$

We have introduced the reduced mass $1/\mu = 1/m_1 + 1/m_2$. H does not depend on the position Q of the center of mass and that is why it commutes with the total momentum. Since P is conserved it can be simultaneously diagonalized with the Hamiltonian

$$P\psi = \frac{\hbar}{i}\partial_Q\psi \Longrightarrow \psi = e^{iPQ/\hbar}\psi(q). \tag{13.6}$$

Let us assume we would like to describe a system with $P = p_1 + p_2 = 0$. We cannot demand this as an operator identity, since this would imply

$$i\hbar = [q_1, p_1] = -[q_1, p_2] = 0,$$

or that the commutation relations are violated. However, we can enforce the constraint $P = 0$ on the physical states,

$$P\psi_{phys} = 0 \Longrightarrow \psi_{phys} = \psi_{phys}(q). \tag{13.7}$$

There is an apparent problem with this procedure, since then

$$\|\psi_{phys}\|^2 = \int dq^1 dq^2 |\psi_{phys}(q)|^2 = \int dQ \int dq\, |\psi_{phys}(q)|^2 = \infty$$

which is a consequence of demanding that physical states have a sharp value of P (which is conjugate to Q). The solution to this problem is that we should not normalize with respect to Q. However one should keep in mind that the physical states are not normalizable, else one could run into formal contradictions as

$$0 = \langle\psi_{phys}|QP - PQ|\psi_{phys}\rangle = i\hbar\langle\psi_{phys}|\psi_{phys}\rangle \neq 0.$$

Now we wish to implement the constraint into the path integral. For doing that it is convenient to use the phase-space formulation of the path integral. This is similarly derived as the path integral (2.29) in the coordinate space. One first introduces the eigenstates of the position and momentum operators:

$$\hat{q}|q\rangle = q|q\rangle \quad \text{and} \quad \hat{p}|p\rangle = p|p\rangle \tag{13.8}$$

obeying the orthogonality conditions

$$\langle q|q'\rangle = \delta(q - q') \quad , \quad \langle p|p'\rangle = 2\pi\hbar\delta(p - p') \tag{13.9}$$

and the completeness relations

$$\int dq|q\rangle\langle q| = \mathbb{1} \quad , \quad \int dp|p\rangle\langle p| = 2\pi\hbar. \tag{13.10}$$

Then inner product of the position and momentum eigenstates are

$$\langle p|q\rangle = e^{-ipq/\hbar}. \tag{13.11}$$

Now we proceed as in the coordinate space and write the evolution kernel as (with the same conventions as in (2.27), e.g. $\tau = it/\hbar$)

$$K(t,q',q) = \langle q'|e^{-itH}|q\rangle = \int dq_1 \dots dq_{n-1} \prod_{j=0}^{n-1} \langle q_{j+1}|e^{-itT/n}e^{-itV/n}|q_j\rangle. \tag{13.12}$$

Each of the factors can be rewritten as

$$\langle q_{j+1}|e^{-itT/n}e^{-itV/n}|q_j\rangle = \int \frac{dp_j}{2\pi\hbar} \langle q_{j+1}|p_j\rangle\langle p_j|e^{-itT/n}e^{-itV/n}|q_j\rangle.$$

The integrand is just

$$\langle q_{j+1}|p_j\rangle\, e^{-it/n\left(T(p_j)+V(q_j)\right)}\langle p_j|q_j\rangle = e^{ip_j(q_{j+1}-q_j)/\hbar - it/n\, H(p_j,q_j)}.$$

where $T(p_j)$ and $V(q_j)$ are the values of the kinetic and potential energy in the momentum and position eigenstates, respectively. Hence their sum $H(p_j,q_j)$ is just the classical energy of a particle with momentum p_j at position q_j. If T also depends on the coordinate this is still true if it is understood that the kinetic energy is normally ordered, that is the momentum on the left and the coordinates on the right. When rewriting each factor this way and reinserting $\hbar$ we finally end up with

$$K(t,q',q) = \lim_{n\to\infty} \int\limits_{q_0=q}^{q_n=q'} \prod_1^{n-1} \frac{dq_i dp_i}{2\pi\hbar} \exp\Big[\frac{i}{\hbar}\sum_1^{n-1}\{p_j(q_{j+1}-q_j) - \epsilon H(p_j,q_j)\}\Big] \tag{13.13}$$

which formally can again be written as

$$K(t,q',q) = \text{const}\cdot \int\limits_{q(0)=q}^{q(t)=q'} \mathcal{D}q\mathcal{D}p \exp\Big[\frac{i}{\hbar}\int \left(p(t)\dot{q}(t) - H[p(t),q(t)]\right)\Big]. \tag{13.14}$$

For a standard kinetic term $T = p^2/2m$ one has

$$\int \frac{dp_j}{2\pi\hbar} \exp\Big[\frac{i}{\hbar}(p_j(q_{j+1}-q_j) - \epsilon\frac{p_j^2}{2m})\Big] = \sqrt{\frac{m}{2\pi i\hbar\epsilon}} \exp\Big\{\frac{im}{2\hbar\epsilon}(q_{j+1}-q_j)\Big\}$$

and thus we recover the representation (2.29) for the path integral in coordinate space,

$$\begin{aligned} K(t,q',q) &= \lim_{n\to\infty}\int dq_1\cdots dq_{n-1}\Big(\frac{m}{2\pi i\hbar\epsilon}\Big)^{n/2} \\ &\qquad \exp\Big\{\frac{i\epsilon}{\hbar}\sum_{j=0}^{j=n-1}\Big[\frac{m}{2}(\frac{q_{j+1}-q_j}{\epsilon})^2 - V(q_j)\Big]\Big\}. \end{aligned} \tag{13.15}$$

Now we would like to express the evolution kernel for the system (13.5) subject to the constraint that the total momentum vanishes, in the full phase space. Clearly, on the physical subspace we have

$$\langle\psi_{phys}|e^{itH}|\psi_{phys}\rangle = \langle\psi_{phys}|e^{itH_{CM}}|\psi_{phys}\rangle$$

such that on this subspace

$$K(t,q',q) = \int \mathcal{D}q\mathcal{D}p\exp\Big[\frac{i}{\hbar}\int\big(p(t)\dot q(t) - H_{CM}[p(t),q(t)]\big)\Big]. \tag{13.16}$$

We wish to integrate not only over the reduced variables but over the full phase space variables. It is not enough to just insert a delta-function $\prod\delta(P_j)$ to implement the constraint into the functional integral since then the $\prod dQ_j$ integrations in

$$\int\mathcal{D}q\mathcal{D}p\mathcal{D}Q\mathcal{D}P\prod\delta(P_j)e^{\frac{i}{\hbar}\sum\big(P_j(Q_{j+1}-Q_j)+p_j(q_{j+1}-q_j)-\epsilon H(P_j,p_j,q_j)\big)}$$

diverges. This can be remedied by inserting another delta-function in the variables Q_j conjugate to the constraint, setting them to arbitrary constants Y_j. Since the Jacobi Matrix of the canonical transformation (13.3) has determinant one and since $P_j(Q_{j+1}-Q_j)+p_j(q_{j+1}-q_j)$ transforms into the same expression with $(P,Q,p,q)\to(p_1,q^1,p_2,q^2)$ we find

$$K(t,q',q) = \text{const}\cdot\int\mathcal{D}q^i\mathcal{D}p_i\;\delta(P)\delta(Q-Y)\exp\Big\{\frac{i}{\hbar}\int\big(p_i\dot q^i - H[p_i,q^i]\big)\Big\},$$

where we have taken the continuum limit such that $\prod\delta(P_j)\to\delta(P(t))\equiv\delta(P)$ and similarly for $\prod\delta(Q_j-Y_j)$. If it is not clear how to identify the variable conjugate to the constraint we may use a delta-function of an arbitrary function of Q and q, provided we recall

$$\prod\delta(Q_j-Y_j) = \prod\delta(F_j(q^i))\det\Big(\frac{\partial F_j}{\partial Q^k}\Big),\qquad (q^i)=(q^1,q^2). \tag{13.17}$$

On the other hand the partial derivative is recognized as the Poisson brackets between the constraint and the function F,

$$\{F_j(q^i),P_k\} = \frac{\partial F_j}{\partial Q^k} \tag{13.18}$$

and thus we arrive at Faddeev's formula for the functional integral on the full 2-body phase space appropriate to a constrained quantum system [50]

$$\begin{aligned} K(t,q',q) &= \int \mathcal{D}q^i\mathcal{D}p_i\; \delta(P)\delta(F)\det\Big(\frac{\delta F(q^i(t))}{\delta Q(t')}\Big)\exp\Big\{\frac{i}{\hbar}\int(p_i\dot q^i - H(p_i,q^i)\Big\} \\ &= \int \mathcal{D}q^i\mathcal{D}p_i\delta(P)\delta(F)\det\{F,P\}\exp\Big\{\frac{i}{\hbar}\int(p_i\dot q^i - H(p_i,q^i)\Big\}. \end{aligned} \tag{13.19}$$

The first delta function enforces the constraint. Since the second one involves an arbitrary function it is called a *choice of gauge*. It follows from our derivation that the path integral is unaffected by a different choice of the auxiliary condition $F(q^i)=0$. Note that the exponent is just the classical action in terms of the canonical variables.

The expression has the following *geometric interpretation:* The constraint $P=0$ defines a 3-dimensional sub-manifold $\mathcal{C}$ (in our simple example it is just a plane, since the constraint is linear) of the 4-dimensional phase space. However, the constraint also generates a Hamiltonian flow,

$$\dot O = \{O,P\} \qquad \text{or} \quad \dot O = \nabla_{X_P}O = X_P^i\partial_i O, \quad \text{where} \quad X_P = J\nabla P, \tag{13.20}$$

and J is the symplectic matrix, $J = i\sigma_2\otimes Id$. Since $\dot P = \{P,P\} = 0$, this is a flow on $\mathcal{C}$. Furthermore, from (13.2) we see that H is constant on the lines of flow in $\mathcal{C}$. Now we can identify two points if and only if they belong to the same trajectory of the flow (13.20). This defines an equivalence relation which is independent of the choice of the constraint (we could have taken an equivalent constraint $a(p,q)\cdot P=0$, where $a(p,q)$ possesses no zeroes, instead of $P=0$) and is invariant under the time evolution. All observables commute (weakly) with the constraint and thus are constant under the flow generated by the constraint. We see that the constraint generates a (gauge) symmetry of the system. It is thus sufficient to choose a representative in each equivalence class in a regular manner. The regularity condition means that one chooses a submanifold of $\mathcal{C}$ by fixing a gauge $F=0$ such that each flow trajectory intersects this sub-manifold exactly once. Locally this is equivalent to demanding that the flow generated by the constraint is never parallel to the gauge-fixing surface $F=0$, or that the inner product of the vector X_P generating the flow and the gradient vector ∇F orthogonal to the gauge fixing surface in $\mathcal{C}$ does not vanish

$$(X_P,\nabla F) = \nabla_{X_P}F = \{F,P\} \neq 0. \tag{13.21}$$

In particular, if one chooses for F the variable conjugate to the constraint, then these vectors are parallel and the gauge fixing surface is orthogonal to the flow trajectories.

The described procedure can be *generalized* to a set of m independent first class constraints in a $2n$-dimensional phase space, that is a set of constraints

$$C_j(p_i,q^i) = 0, \qquad j=1,\dots,m, \tag{13.22}$$

which form a closed algebra and weakly commute with the Hamiltonian,

$$\{C_i, C_j\} = a_{ijk}(p_i, q^i)C_k \quad \text{and} \quad \{H, C_i\} = a_{ij}C_j, \tag{13.23}$$

They define a $2n - m$ dimensional submanifold $\mathcal{C}$ of the phase space. The flows generated by these constraints stay entirely in $\mathcal{C}$ and are symmetries of the system. Again one chooses a regular gauge

$$F_i(p_i, q^i) = 0, \quad i = 1, .., m, \qquad \det\{F_i, C_j\} \neq 0, \tag{13.24}$$

which defines a $2(n - m)$ dimensional sub-space of the full phase space which may in turn be considered as a phase space. Similar considerations as above lead to the same path integral representation for $K(t, q', q)$ as given by (13.19), where now $\delta(P)$ is replaced by $\prod \delta(C_i)$ and $\delta(F)$ by $\prod \delta(F_i)$.