Chapter 13 General Aspects of Effective Descriptions

Effective actions or equations are always a powerful tool to analyze general effects of a quantum theory. They can be difficult to derive, but once obtained at least in an approximate form they allow detailed studies and provide more intuition than what can be obtained from dealing with wave functions. Key for their derivation is the availability of a simple solvable model in which quantum properties can be obtained in an exact and compact form. In quantum mechanics, this sovable model is the harmonic oscillator, which in the form of free field theories also appears as the firm solvable basis for quantum field theory on a background space-time. Perturbation theory around the solvable model allows one to include anharmonicities, interactions or extra fields. The harmonic cosmology of a free massless scalar in a flat, isotropic universe plays the solvable role for quantum cosmology.

13.1 Canonical Effective Equations

For a canonical quantization such as loop quantum cosmology we have to use a Hamiltonian way of deriving effective equations. We start with a *-algebra \mathscr{A} of operators, possibly together with a representation on a Hilbert space \mathscr{H} . A representation would help us in dealing with pure states, but our discussion here will be at the general level of density states which may be mixed. We will focus on operators whose algebra, rather than representation, turns out to be more important; most statements in this chapter are representation-independent. (The algebra of observables is crucial. We will be able to distinguish between a Wheeler–DeWitt quantization and a loop quantization because the latter contains only holonomies of connection components which obey different algebraic relations with fluxes. Once the algebra of operators is fixed, crucial consequences are captured independently of whether a Schrödinger or Bohr representation is introduced.)

13.1.1 States and Moments

A state is a positive linear functional $\omega: \mathscr{A} \to \mathbb{C}$ on the *-algebra, that is a linear functional satisfying $\omega(\hat{A}^*\hat{A}) \geq 0$ for all $\hat{A} \in \mathscr{A}$ as well as $\omega(\hat{A}^*) = \omega(\hat{A})^*$. (The latter property can be derived if the algebra is unital, as we normally assume.) One example is a pure state ψ in a Hilbert-space representation of \mathscr{A} , for which $\omega_{\psi}(\hat{A}) = \langle \psi, \hat{A}\psi \rangle$, or a density matrix ρ for which $\omega_{\rho}(\hat{A}) = \text{tr}(\hat{A}\rho)$. The notion of states allows us to view observables in the algebra \mathscr{A} in a "classical" way as functions on a phase space. We first introduce the space on which these functions are defined as the space \mathscr{P} of all states ω on the algebra. Any element A of the algebra then defines a function $\langle \hat{A} \rangle : \mathscr{P} \to \mathbb{C}, \omega \mapsto \omega(\hat{A})$. As the notation indicates, this function is nothing but the expectation-value functional associated with \hat{A} .

13.1.2 Quantum Phase Space

Classical observables are real-valued functions on the phase space. Accordingly, we require that quantum observables \hat{O} provide real expectation-value functionals $\langle \hat{O} \rangle$, a large class being self-adjoint ones: $\hat{O}^* = \hat{O}$. Moreover, classical observables are functions on a phase space, which is equipped with a Poisson bracket. For expectation-value functionals, we introduce

$$\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\} = \frac{\langle [\hat{A}, \hat{B}] \rangle}{i\hbar}.$$
(13.1)

For functions obtained as products or other expressions in terms of expectationvalue functions, we extend the Poisson bracket using linearity and the Leibniz rule. It follows from the properties of the commutator that this is indeed a Poisson bracket. (Note that we define the Poisson bracket by (13.1). It is not required to equal the classical Poisson bracket for all expressions corresponding to \hat{A} and \hat{B} . In general, it will be identical to the classical Poisson bracket only if \hat{A} and \hat{B} are basic operators.)

For explicit calculations, it is often most useful to choose coordinates. There is a natural choice if we have a distinguished set of basic operators in our algebra, which form a closed subalgebra under taking commutators and which can be used to generate all other elements in the algebra by their products. For quantum mechanics, these basic operators would usually be taken as the position and momentum operators \hat{q} and \hat{p} with $[\hat{q}, \hat{p}] = i\hbar$, but one may use other versions such as $e^{i\mu c/2}$ and \hat{p} with $[e^{i\mu c/2}, \hat{p}] = -\frac{4}{3}\pi\gamma \ell_{\rm P}^2\mu e^{i\mu c/2}$ in loop quantum cosmology, or entire smeared field algebras in quantum field theory and the holonomy-flux algebra in loop quantum gravity.

Let us assume that we have a set of basic operators \hat{J}_i , i = 1, 2, ..., N, which is linear and closed under taking commutators: $[\hat{J}_i, \hat{J}_j] = i\hbar C_{ij}^k \hat{J}_k$. (For a canonical algebra, we allow the identity $\hat{J} = \hat{I}$ as a possible basic operator.) Expectationvalue functionals of the basic operators then satisfy the same Poisson algebra: $\{\langle \hat{J}_i \rangle, \langle \hat{J}_j \rangle\} = C_{ij}^k \langle \hat{J}_k \rangle$. But they do not provide a complete set of coordinates on the space of all functions on \mathscr{P} because in general we have $\langle \hat{J}_i \hat{J}_j \rangle \neq \langle \hat{J}_i \rangle \langle \hat{J}_j \rangle$, and no other general relation between $\langle \hat{J}_i \hat{J}_j \rangle$ or other expectation values of products and the basic expectation values of \hat{J}_i exists. In fact, even if the basic algebra is finite, as in quantum mechanics or homogeneous models of quantum cosmology, the space of states is usually infinite-dimensional. (Exceptions are cyclic finitely generated algebras as they occur for spin systems; see the examples below.) Expectation-value functionals of products of the basic operators, called moments, provide the remaining coordinates. Unless there are non-trivial relations between operators in the algebra, all moments of density states are independent and in fact of infinite number.

It is convenient to define moments not directly as expectation-value functionals of products of basic operators but in the form already introduced in (5.23):

$$\Delta(O_1 O_2 \cdots O_n) := \left\langle (\hat{O}_1 - \langle \hat{O}_1 \rangle) (\hat{O}_2 - \langle \hat{O}_2 \rangle) \cdots (\hat{O}_n - \langle \hat{O}_n \rangle) \right\rangle_{\text{symm}}$$
$$= \frac{1}{n!} \sum_{\pi \in S_n} \left\langle (\hat{O}_{\pi(1)} - \langle \hat{O}_{\pi(1)} \rangle) (\hat{O}_{\pi(2)} - \langle \hat{O}_{\pi(2)} \rangle) \cdots (\hat{O}_{\pi(n)} - \langle \hat{O}_{\pi(n)} \rangle) \right\rangle$$
(13.2)

where we totally symmetrize to remove redundancy due to re-ordering. (Moreover, symmetrization makes the moments real provided the \hat{O}_i used are self-adjoint.) These moments are non-trivial only for $n \ge 2$ since $\langle (\hat{O} - \langle \hat{O} \rangle) \rangle = 0$ for normalized states. At second order, we use the standard notation $(\Delta O)^2 = \Delta (O^2)$.

With this choice of moments, it is guaranteed that expectation-value functionals of the basic operators Poisson commute with their moments: $\{\langle \hat{O} \rangle, \Delta(O_1 O_2 \ldots)\} = 0$ provided the basic operators \hat{O} , \hat{O}_1 and \hat{O}_2 satisfy a canonical algebra. This property often provides computational advantages, but even for non-canonical basic operators the choice of moments in this form is useful because they are all expected to be small in a semiclassical state, or vanish in a classical correspondence. In this limit only the basic expectation values remain and correspond to classical variables. Accordingly, the moments (5.23) are sometimes called quantum variables. For the general Poisson bracket of moments for canonical basic operators, see [1].

13.1.3 Relations

With expectation-value functionals and the moments we have a complete set of coordinates on the state space. But the moments cannot take arbitrary real values: Fluctuations of the form $(\Delta O)^2 = \langle (\hat{O} - \langle \hat{O} \rangle)^2 \rangle$ must clearly be non-negative, but in general they are restricted even more strongly by uncertainty relations. For each pair (\hat{O}_1, \hat{O}_2) of operators we have the Schwarz inequality

$$\langle \hat{\Delta} O_1^* \hat{\Delta} O_1 \rangle \langle \hat{\Delta} O_2^* \hat{\Delta} O_2 \rangle \ge |\langle \hat{\Delta} O_1^* \hat{\Delta} O_2 \rangle|^2$$

with $\hat{\Delta}O_i := \hat{O}_i - \langle \hat{O}_i \rangle$. If the operators are self-adjoint, this means

$$\langle (\hat{\Delta}O_1)^2 \rangle \langle (\hat{\Delta}O_2)^2 \rangle \ge |\langle \hat{\Delta}O_1 \hat{\Delta}O_2 \rangle|^2.$$
(13.3)

Writing

$$\hat{\Delta}O_1\hat{\Delta}O_2 = \frac{1}{2}(\hat{\Delta}O_1\hat{\Delta}O_2 + \hat{\Delta}O_2\hat{\Delta}O_1) + i\frac{1}{2i}[\hat{\Delta}O_1, \hat{\Delta}O_2]$$

with

$$\frac{1}{2}\langle\hat{\Delta}O_1\hat{\Delta}O_2+\hat{\Delta}O_2\hat{\Delta}O_1\rangle=\frac{1}{2}\langle\hat{O}_1\hat{O}_2+\hat{O}_2\hat{O}_1\rangle-\langle\hat{O}_1\rangle\langle\hat{O}_2\rangle$$

and $[\hat{\Delta}O_1, \hat{\Delta}O_2] = [\hat{O}_1, \hat{O}_2]$ we have

$$|\langle \hat{\Delta} O_1 \hat{\Delta} O_2 \rangle|^2 = \frac{1}{4} \left(\langle \hat{O}_1 \hat{O}_2 + \hat{O}_2 \hat{O}_1 \rangle^2 - 2 \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle \right)^2 + \frac{1}{4} \langle -i[\hat{O}_1, \hat{O}_2] \rangle^2.$$

Again, we have used self-adjointness of the operators to compute the absolute square of the complex number $\langle \hat{\Delta} O_1 \hat{\Delta} O_2 \rangle$. For the moments, we thus have the inequalities

$$(\Delta O_1)^2 (\Delta O_2)^2 - \Delta (O_1 O_2)^2 \ge \frac{1}{4} \langle -i[\hat{O}_1, \hat{O}_2] \rangle^2$$
(13.4)

as uncertainty relations whenever \hat{O}_1 and \hat{O}_2 are self-adjoint. Similar conditions exist for moments of higher order, but they mix the order and are more tedious to derive.

Usually, $[\hat{O}_1, \hat{O}_2] \sim \hbar$. Near the saturation of the uncertainty relation, secondorder moments are thus of the order \hbar , as realized for instance for Gaussian states of canonical quantum systems (see the example below). In that case, $\Delta(O_1 \cdots O_n) \sim O(\hbar^{n/2})$ provides a suitable condition for semiclassicality much wider than one using Gaussians or any specific class of wave functions.

Example 13.1 For the basic operators \hat{q} and \hat{p} represented as the usual operators on the Hilbert space of square-integrable functions of $q \in \mathbb{R}$, pure Gaussian states have the general form $\psi(q) = \exp(-z_1q^2 + z_2q + z_3)$ with three complex numbers z_i such that $\operatorname{Re} z_1 > 0$ for normalizability. The parameter z_3 is irrelevant for the moments since its real part is fixed by normalization while its imaginary part contributes only a phase factor. Writing $z_1 = \alpha_1 + i\beta_1$ and $z_2 = \alpha_2 + i\beta_2$ with real α_i and β_i , we have

$$\langle \hat{q} \rangle = \frac{\alpha_2}{2\alpha_1}, \quad \langle \hat{p} \rangle = \hbar \frac{\alpha_1 \beta_2 - \alpha_2 \beta_1}{\alpha_1},$$
(13.5)

$$(\Delta q)^2 = \frac{1}{4\alpha_1}, \quad (\Delta p)^2 = \hbar^2 \alpha_1 + \hbar^2 \frac{\beta_1^2}{\alpha_1}, \quad \Delta(qp) = -\hbar \frac{\beta_1}{2\alpha_1}$$
(13.6)

characterizing the peak position, fluctuations and correlations of the state. For all allowed values of the parameters, Gaussian states saturate the uncertainty relation

$$(\Delta q)^2 (\Delta p)^2 - \Delta (qp)^2 = \frac{1}{4}\hbar^2.$$
 (13.7)

For $\beta_1 = \text{Im}z_1 \neq 0$, the state is correlated. In this case, the uncertainty product $(\Delta q)^2 (\Delta p)^2$ is larger than the minimally possible value $\hbar^2/4$. Correlations $\Delta(qp)$ are bounded from above for given values of fluctuations Δq and Δp . These are all the moments that can be varied for a Gaussian state; such states are thus much more special than general semiclassical ones.

With (13.2), we are considering moments for general density states. If moments are desired only for pure states of some type, further conditions arise which are complicated to derive completely. Fortunately, such a restriction is rarely necessary. Especially for quantum cosmology which constitutes models obtained by averaging inhomogeneous configurations, density states should be expected to be relevant for sufficient generality.

The preceding example illustrates that none of the second-order moments for a canonical algebra of basic operators is redundant even for pure states: At saturation we have one relation between the three variables, and there are indeed two free parameters in a Gaussion once the expectation values of \hat{q} and \hat{p} are fixed. The third independent moment then enters as a free parameter to describe deviations from saturation. Such unsaturated states, however, are more difficult to write down in closed form with specific moments; they are certainly no longer Gaussian. The following examples illustrate the relationship between moments and density states.

Example 13.2 Take the algebra M_2 of complex 2 × 2-matrices, with an adjoint defined in the usual way by transposition combined with complex conjugation. Self-adjoint generators can be taken to be the Pauli matrices σ_i together with the identity id. There are relations $id\sigma_i = \sigma_i = \sigma_i$ id and $\sigma_i \sigma_j = \delta_{ij} + \varepsilon_{ijk}\sigma_k$ between them such that any product can be reduced to an expression linear in the generators. That means that expectation values of matrices in the set {id, σ_i } as basic operators are sufficient to parameterize all expectation values, and no independent moments exist. Disregarding the trivial unit which must always have the same expectation value one, the quantum phase space is thus three-dimensional—in accordance with the fact that 2 × 2 density matrices have three free parameters. (They are self-adjoint and of trace one.) An irreducible Hilbert-space representation \mathcal{H}_2 , on the other hand, provides a two-dimensional state space: the usual spin-1/2 representation is complex two-dimensional, which with normalization and factoring out a total phase corresponds to two real dimensions. In this simple example, we thus see that the state space we obtain by expectation values and moments is larger than the space of pure states.

Example 13.3 Now take the tensor product $M_2 \otimes M_2$ of the algebra M_2 with itself. It has 16 generators {id \otimes id, id $\otimes \sigma_i$, $\sigma_j \otimes$ id, $\sigma_k \otimes \sigma_l$ }. Again, all products can be reduced to expressions linear in the generators, and disregarding the unit we obtain a 15-dimensional state space in accordance with the dimension of the space of self-adjoint, trace one, 4×4 density matrices. An irreducible Hilbert-space representation $\mathscr{H}_2 \otimes \mathscr{H}_2$, on the other hand, is complex four-dimensional, implying six real dimensions for the pure state space.

13.1.4 Casimir Conditions

Further conditions may arise if several irreducible representations exist for a given linear system $[\hat{J}_i, \hat{J}_j] = i\hbar C_{ij}^k \hat{J}_k$. For instance, one may specify values of Casimirs for group coherent states, such as $\hat{C} := \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2 = \hbar^2 j (j + 1)$ for SU(2) with $C_{ij}^k = \varepsilon_{ij}^k$. Taking an expectation value of the operator equation then relates expectation values of the basic operators to second-order moments (for a quadratic Casimir), and provides relations for higher moments from expectation values of the form

$$\langle \hat{J}_{1}^{k} \hat{J}_{2}^{l} \hat{J}_{3}^{m} \hat{C} \rangle = \hbar^{2} j (j+1) \langle \hat{J}_{1}^{k} \hat{J}_{2}^{l} \hat{J}_{3}^{m} \rangle.$$
(13.8)

Evaluations of these relations then follow the lines as in the example of reality conditions for harmonic loop quantum cosmology used in Sect. 6.1, which amount to a Casimir condition for the algebra $sl(2, \mathbb{R})$.

One may view the Casimir operator as a constraint operator and deal with it along the lines of effective constraints to be described in Sect. 13.2 for first-class constraints. In contrast to the procedure described there, however, a Casimir constraint is second class, even if it is a single constraint. In such a case, it amounts to a constraint on a nonsymplectic Poisson manifold (with degenerate Poisson tensor) for which constraints are classified in a generalized way compared to Dirac's well-known procedure; see [2]. A Casimir constraint, by definition, commutes with all basic operators: $[\hat{J}_i, \hat{C}] = 0$. In the quantum phase space, it does not generate any gauge transformations, a property that distinguishes second-class constraints.

13.1.5 Equations of Motion

On the state space parameterized by expectation values and moments, a flow is defined once a Hamiltonian operator in the algebra \mathscr{A} has been chosen. For expectation values of arbitrary time-independent operators \hat{O} , we have the well-known equation

$$\frac{\mathrm{d}\langle\hat{O}\rangle}{\mathrm{d}t} = \frac{\langle[\hat{O},\hat{H}]\rangle}{\mathrm{i}\hbar}$$
(13.9)

which can be derived equally well in a Schrödinger or Heisenberg picture. Such an equation also applies to evolving observables in deparameterized systems, as seen in the preceding chapter; (12.6). Using linearity and the Leibniz rule of derivatives we extend the dynamics to all moments, for instance

$$\frac{\mathrm{d}(\Delta O)^2}{\mathrm{d}t} = \frac{\mathrm{d}(\langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2)}{\mathrm{d}t} = \frac{\langle [\hat{O}^2, \hat{H}] \rangle}{\mathrm{i}\hbar} - 2\langle \hat{O} \rangle \frac{\langle [\hat{O}, \hat{H}] \rangle}{\mathrm{i}\hbar}.$$
 (13.10)

Example 13.4 (*Harmonic oscillator*) With $\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2$ in the Schrödinger representation, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{q}\rangle = \frac{1}{m}\langle\hat{p}\rangle, \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = -m\omega^2\langle\hat{q}\rangle$$

which can be solved easily and in closed form independently of any moment. Solutions agree exactly with the classical ones, as is well known from the Ehrenfest theorem. Similarly, the second-order moments satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}(\Delta q)^2 = \frac{2}{m}\Delta(qp)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\Delta(qp) = -m\omega^2(\Delta q)^2 + \frac{1}{m}(\Delta p)^2$$
$$\frac{\mathrm{d}}{\mathrm{d}t}(\Delta p)^2 = -2m\omega^2\Delta(qp)$$

and can also be solved for in closed form without knowing any higher moment. Second-order moments, moreover, are subject to the (generalized) uncertainty relation

$$(\Delta q)^2 (\Delta p)^2 - \Delta (qp)^2 \ge \frac{\hbar^2}{4}$$

The second-order equations allow one to discuss coherent and squeezed states in simple terms. We have non-spreading solutions of constant second-order moments provided that $\Delta(qp) = 0$, $\Delta p = m\omega\Delta q$. All these solutions correspond to coherent states following exactly the classical trajectory. They satisfy the uncertainty relation if $\Delta q \geq \sqrt{\hbar/2m\omega}$. If the uncertainty relation is saturated, we obtain fluctuations that are fixed uniquely to be those of the ground state. If we saturate the uncertainty relation at all times, we have general dynamical coherent states. From the previous equations, this implies fluctuations changing in time unless we have exactly the harmonic oscillator ground state; such states are called squeezed states. See Fig. 13.1 for an illustration. In their most general form, squeezed states may also have nonvanishing correlations if $\Delta(qp) \neq 0$. For given fluctuations, however, the amount of squeezing is bounded by the uncertainty relation $|\Delta(qp)| \leq \sqrt{(\Delta q)^2 (\Delta p)^2 - \hbar^2/4}$ even if it is not required to be saturated.

Dynamics is more involved for anharmonic systems, in which the equations of motion for all infinitely many moments no longer decouple to finitely coupled sets of linear equations. In this case, quantum back-reaction results and the precise behavior of an evolving state, including its spreading and deformations from a Gaussian, is important for knowing the time dependence of expectation values or other moments. It is generated by the quantum Hamiltonian

$$H_Q = \langle H(\hat{q}, \hat{p}) \rangle = \langle H(q + (\hat{q} - q), p + (\hat{p} - p)) \rangle$$
(13.11)

$$= H(\langle \hat{q} \rangle, \langle \hat{p} \rangle) + \sum_{a,b} \frac{1}{a!b!} \frac{\partial^{a+b} H(\langle \hat{q} \rangle, \langle \hat{p} \rangle)}{\partial \langle \hat{q} \rangle^a \partial \langle \hat{p} \rangle^b} \Delta(q^a p^b).$$
(13.12)



The expansion in terms of the moments, just as a semiclassical \hbar -expansion used for the WKB approximation, or like the Feynman expansion, is in general not convergent but asymptotic. The equations of motion $\dot{f} = \{f, H_Q\}$ it generates follow from the Poisson bracket in the quantum phase space. Its relationship to commutators then shows that H_Q generates the correct flow for expectation values and moments based on (13.9).

In canonical formulations, the Hamiltonian determines the dynamics together with the Poisson structure. One could therefore suspect that not only the Hamiltonian but also the Poisson brackets receive quantum corrections. This suspicion is correct: The Poisson structure receives corrections by the presence of moments as new quantum degrees of freedom, enlarging the classical phase space. However, by definition (13.1) there are no quantum corrections to the basic variables as long as they form a closed algebra (belonging to a linear quantum system). The Poisson brackets of expectation values of basic operators agree with the classical Poisson brackets, without quantum corrections in this relation.

If one does not work with the full Poisson manifold of expectation values and all moments, but rather embeds the classical phase space non-horizontally in the quantum phase space seen as a fiber bundle over the classical phase space, quantum corrections to Poisson brackets of expectation values do arise. For instance, in the following example we will see that under certain conditions (more precisely, when an adiabatic approximation can be applied for the moments) one can solve for the moments $\Delta(q^a p^b)(\langle \hat{q} \rangle, \langle \hat{p} \rangle)$ in terms of the expectation values. These solutions then describe an embedding $(q, p) \mapsto (q, p, \Delta(q^a p^b)(q, p))$ of the classical phase space in the quantum phase space. If one pulls back the symplectic form $d\langle \hat{q} \rangle \wedge d\langle \hat{p} \rangle + \Omega_{a,b;c,d}(\Delta) \Delta \Delta(q^a p^b) \wedge d\Delta(q^c p^d)$ on the quantum phase space (with moment-dependent coefficients encoding the Poisson structure (13.1) for moments), one may obtain a quantum-corrected symplectic form

$$(1+2\Omega_{a,b;c,d}(\Delta(q,p))(\partial\Delta(q^ap^b)/\partial q)(\partial\Delta(q^cp^d)/\partial p))\mathrm{d}q\wedge\mathrm{d}p.$$

(Such a correction does not arise in the following example because the moments solved for in terms of expectation values depend only on $\langle \hat{q} \rangle$, not on $\langle \hat{p} \rangle$.) Sometimes, corrections of this form also arise when one begins the derivation of effective equations by an assumption on, rather than derivation of, the dependence of moments on expectation values, as in [3].

Thus, if quantum corrections to the symplectic or Poisson structure arise, they are a consequence of a secondary step in solving effective equations or making assumptions about their solutions. If moments are kept independent of expectation values, which is the most general form of effective equations, no corrections to the Poisson brackets of expectation values arise, while Poisson brackets between moments as they follow from commutators have no classical analog whatsoever.

The infinitely-coupled dynamics of ordinary differential equations for moments is equivalent to the partial differential equation given by the Schrödinger flow. Usually, the Schrödinger equation is much more useful for solving the dynamics. But in certain regimes, equations for moments lend themselves more easily to approximation schemes.

Example 13.5 (*Anharmonic oscillator*) With a cubic anharmonicity in the Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2 + \frac{1}{3}\lambda\hat{q}^3$$

we have equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{q}\rangle = \frac{1}{m}\langle\hat{p}\rangle, \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = -m\omega^2\langle\hat{q}\rangle - \lambda\langle\hat{q}\rangle^2 - \lambda(\Delta q)^2$$

with a non-linear coupling of expectation values and the q-fluctuation. To solve these equations, we must know the behavior of Δq , which is itself time dependent with a rate of change

$$\frac{\mathrm{d}}{\mathrm{d}t}(\Delta q)^2 = \frac{2}{m}C_{qp} \tag{13.13}$$

given by the covariance, obeying

$$\frac{\mathrm{d}}{\mathrm{d}t}C_{qp} = \frac{1}{m}C_{qp} + m\omega^2(\Delta q)^2 + 6\lambda\langle\hat{q}\rangle(\Delta q)^2 + 3\lambda\Delta(q^3).$$
(13.14)

Here, a higher moment $\Delta(q^3)$ of third order couples. Proceeding this way in the hope of finding a closed set of equations, one will have to include all infinitely many moments.

For a general anharmonic system, we consider a classical Hamiltonian $H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2q^2 + U(q)$. In this case, additional approximation schemes open up which will allow us to compare results with other derivations based, for instance, on effective actions. Using the parameters of the anharmonic system, we first introduce dimensionless variables $\tilde{\Delta}(q^b p^a) := \hbar^{-(a+b)/2}(m\omega)^{b/2-a/2}\Delta(q^b p^a)$. The quantum Hamiltonian, including coupling terms between expectation values and moments, can then be expanded in powers of $\hbar^{1/2}$:

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$$H_{Q}(\langle \hat{q} \rangle, \langle \hat{p} \rangle, \Delta(\cdots)) = \frac{1}{2m} \langle \hat{p} \rangle^{2} + \frac{1}{2} m \omega^{2} \langle \hat{q} \rangle^{2} + U(\langle \hat{q} \rangle) + \frac{\hbar \omega}{2} \left((\tilde{\Delta}q)^{2} + (\tilde{\Delta}p)^{2} \right) + \sum_{n>2} \frac{1}{n!} \left(\frac{\hbar}{m\omega} \right)^{n/2} U^{(n)}(\langle \hat{q} \rangle) \tilde{\Delta}(q^{n}).$$
(13.15)

Here the dimensionless variables are useful to organize the formal expansion with an explicit expansion parameter \hbar . In general, such expansions can still be performed if one assumes the moments to obey the semiclassical hierarchy $\Delta(q^a p^b) \sim O(\hbar^{(a+b)/2})$. With the dimensionless moments, we have $\tilde{\Delta}(q^a p^b) \sim O(1)$ and all orders of \hbar are indeed shown explicitly in (13.15). From this expression, we see the zero-point energy given just by the fluctuations, $(\tilde{\Delta}q)^2 = (\tilde{\Delta}p)^2 = 1/2$ for the ground state, and quantum back-reaction from coupling terms between expectation values and moments.

Equations of motion then follow in the usual Hamiltonian way as $\dot{f} = \{f, H_Q\}$ for any phase-space function f, using the Poisson brackets as defined in (13.1) together with linearity and the Leibniz rule. One can easily see that the resulting equations agree with what we had earlier obtained by the background-state method in Sect. 5.4.1, expanding the Hamiltonian operator directly but formally. For the anharmonic oscillator, we have

$$\langle \dot{\hat{q}} \rangle = \frac{\langle \hat{p} \rangle}{m} \tag{13.16}$$

$$\begin{split} \langle \dot{\hat{p}} \rangle &= -m\omega^{2} \langle \hat{q} \rangle - U'(\langle \hat{q} \rangle) - \sum_{n} \frac{1}{n!} \left(\frac{\hbar}{m\omega} \right)^{n/2} U^{(n+1)}(\langle \hat{q} \rangle) \tilde{\Delta}(q^{n}) \quad (13.17) \\ \dot{\tilde{\Delta}}(q^{n-a}p^{a}) &= -a\omega\tilde{\Delta}(q^{n-a+1}p^{a-1}) + (n-a)\omega\tilde{\Delta}(q^{n-a-1}p^{a+1}) \\ &- a \frac{U''(\langle \hat{q} \rangle)}{m\omega} \tilde{\Delta}(q^{n-a+1}p^{a-1}) \\ &+ \frac{\sqrt{\hbar}aU'''(\langle \hat{q} \rangle)}{2(m\omega)^{\frac{3}{2}}} \tilde{\Delta}(q^{n-a}p^{a-1}) \tilde{\Delta}(q^{2}) + \frac{\hbar aU''''(\langle \hat{q} \rangle)}{3!(m\omega)^{2}} \tilde{\Delta}(q^{n-a}p^{a-1}) \tilde{\Delta}(q^{3}) \\ &- \frac{a}{2} \left(\frac{\sqrt{\hbar}U'''(\langle \hat{q} \rangle)}{(m\omega)^{\frac{3}{2}}} \tilde{\Delta}(q^{n-a+2}p^{a-1}) + \frac{\hbar U''''(\langle \hat{q} \rangle)}{3(m\omega)^{2}} \tilde{\Delta}(q^{n-a+3}p^{a-1}) + \cdots \right) \\ &+ \frac{a(a-1)(a-2)}{24} \left(\frac{\sqrt{\hbar}U'''(\langle \hat{q} \rangle)}{(m\omega)^{\frac{3}{2}}} \tilde{\Delta}(q^{n-a}p^{a-3}) \\ &+ \frac{\hbar U''''(\langle \hat{q} \rangle)}{(m\omega)^{2}} \tilde{\Delta}(q^{n-a+1}p^{a-3}) + \cdots \right). \end{split}$$

As expected, these are infinitely many coupled equations for infinitely many variables. (Incidentally, note that the expansion is in terms of $\sqrt{\hbar}$, not of \hbar as one might have expected. Half-integer powers of \hbar only drop out if all odd-order moments vanish, which is the case for harmonic oscillator coherent states but not necessarily in general.)

Solving these equations even approximately requires truncations that allow one to disregard all but finitely many moments. The set of moments indeed has the hierarchy of finite-dimensional spaces \mathscr{P}_n defined as the subsets obtained by allowing moments $\Delta(q^a p^b)$ only up to a finite order $a + b \leq n$. Commutators do not directly provide a closed Poisson bracket on these spaces; for instance, at third order we have $\{\Delta(q^3), \Delta(p^3)\} = 9(\Delta(q^2p^2) - (\Delta q)^2(\Delta p)^2)$ which includes a moment of order four. (Only second-order moments have a closed Poisson algebra among themselves.) But truncating not only the Hamiltonian but also the Poisson brackets at a finite order *n* provides the dynamics on a closed Poisson manifold. That this truncation also of the Poisson brackets is in fact required for a consistent approximation of equations of motion can be seen from the observation that it results in a Hamiltonian flow corresponding exactly to the equations of motion truncated at the same order *n*.

There is thus a consistent truncation procedure which in terms of dimensionless moments disregards all terms beyond a certain order $\hbar^{n/2}$. Here, the expansion is a semiclassical one, but formally one can do similar truncations in other regimes. To that end, we would replace each moment $\Delta(q^a p^b)$ with $\mu^{(a+b)/2} \Delta(q^a p^b)$ and \hbar with $\mu\hbar$, expand all equations up to terms of order $\mu^{n/2}$ (irrespective of the value of \hbar). After setting $\mu = 1$, we obtain the truncated equations.

In general, the truncation results in a higher-dimensional dynamical system in which the expectation values are accompanied by some of the moments as true quantum degrees of freedom. By the coupling terms among the equations, quantum back-reaction is realized. Sometimes one can further reduce the system to one of the classical dimension, involving only expectation values, such that quantum back-reaction is realized in a simpler way, for instance by an effective potential. Such an additional step requires solutions to some of the equations for moments in terms of expectation values, which can then be inserted into the expectation-value equations. For the anharmonic oscillator, this is possible by an adiabatic approximation for the moments which indeed allows one to solve the moment equations without knowing the behavior of expectation values, and then insert the solutions into the coupling terms of expectation-value equations.

Performing an adiabatic approximation again makes use of a formal parameter λ to arrange expansions, and in the end setting $\lambda = 1$. Now, a small value of the parameter should mean that the time dependence of moments is only weak. We thus rescale d/dt to $\lambda d/dt$ and expand $\Delta(q^a p^b) = \sum_e \Delta_e(q^a p^b)\lambda^e$. After solving the equations order by order in λ , we will finally set $\lambda = 1$. There is no claim that the λ -expansion of $\Delta(\cdots)$ is a converging sum, and the procedure might seem questionable. Instead, the expansion merely serves to organize different kinds of time dependences of the moments. To *n*-th adiabatic order, comparing λ -coefficients in the adiabatic expansion of the general Hamiltonian equation of motion leads to

$$\{\Delta_n(q^a p^b), H_Q\} = \dot{\Delta}_{n-1}(q^a p^b).$$
(13.19)

(Writing this equation as $\{\Delta_n(q^a p^b) - \Delta_{n-1}(q^a p^b), H_Q\} = 0$ shows that at *n*-th adiabatic order the highest-order term is assumed to provide a contribution of negligibly small time dependence to the expansion of moments.) Iterating (13.19) over *n*, with the left-hand side computed as a Poisson bracket on phase space rather than interpreted as a time derivative, this procedure provides algebraic equations to all orders. We will see this explicitly when we apply these equations to the anharmonic oscillator.

To first order in \hbar and zeroth in λ , we have from (13.18) without the \hbar -terms and without the time derivative (which is at least of first order in λ) [4]

$$0 = (n-a)\tilde{\Delta}_0(q^{n-a-1}p^{a+1}) - a\left(1 + \frac{U''(\langle \hat{q} \rangle)}{m\omega^2}\right)\tilde{\Delta}_0(q^{n-a+1}p^{a-1}).$$
 (13.20)

As a step-2 recurrence in *a* for $\tilde{\Delta}_0(q^{n-a}p^a)$ starting with $\tilde{\Delta}_0(q^n)$, (13.20) must stop at a = n since the sequence of *n*-th order moments is finite. Non-zero solutions of this form can arise only if n = a is the last step in the recursion, which implies that *a* must be even for even *n* and odd for odd *n*. For even *n* and *a* we have the general solution

$$\tilde{\Delta}_0(q^{n-a}p^a) = \binom{n/2}{a/2} \binom{n}{a}^{-1} \left(1 + \frac{U''(\langle \hat{q} \rangle)}{m\omega^2}\right)^{a/2} \tilde{\Delta}_0(q^n),$$
(13.21)

and we will not need the odd-order solutions. To this order, $\overline{\Delta}_0(q^n)$ remains free. To first order in λ , we have

$$(n-a)\tilde{\Delta}_{1}(q^{n-a-1}p^{a+1}) - a\left(1 + \frac{U''(\langle \hat{q} \rangle)}{m\omega^{2}}\right)\tilde{\Delta}_{1}(q^{n-a+1}p^{a-1}) = \frac{1}{\omega}\dot{\tilde{\Delta}}_{0}(q^{n-a}p^{a})$$

which implies

$$\sum_{a \text{ even}} \binom{n/2}{a/2} \left(1 + \frac{U''(\langle \hat{q} \rangle)}{m\omega^2} \right)^{(n-a)/2} \dot{\tilde{\Delta}}_0(q^{n-a}p^a) = 0$$

for consistency. This condition requires

$$\tilde{\Delta}_0(q^n) = C_n (1 + U''(\langle \hat{q} \rangle) / m\omega^2)^{-n/4}$$
(13.22)

with constants C_n . At this stage, we see that the zeroth-order adiabatic solutions are not *t*-independent but implicitly depend on *t* via $\langle \hat{q} \rangle$ if the potential is not quadratic. The equation (13.20) we solved therefore cannot provide an exact solution to (13.18): Higher orders in the adiabatic approximation correct for this error in the time dependence; this reorganization of the *t*-dependence is the actual meaning of the formal λ -expansion.

To obtain moments of the ground state for the harmonic limit U = 0, we must have $C_n = 2^{-n} n! / (n/2)!$ (as well as $\tilde{\Delta}(q^{n-a} p^a) = 0$ for *a* and *n* odd, which is why we do not need the solution of (13.20) for such values). The zeroth adiabatic order for second-order moments is then fixed completely, and we obtain the first correction

$$\dot{p} = -m\omega^2 q - U'(q) - \frac{\hbar}{2m\omega}U'''(q)(\tilde{\Delta}_0 q)^2 + \cdots$$
$$= -m\omega^2 q - U'(q) - \frac{\hbar}{4m\omega}\frac{U'''(q)}{\sqrt{1 + U''(q)/m\omega^2}} + \cdots$$

to the classical equations of motion. The last term shows the leading correction in the effective force as compared to the classical force -U'(q) from the effective potential in H_Q with the zero-point energy.

To second adiabatic order [4] we obtain additional corrections, which imply the second-order equation of motion

$$\begin{split} &\left(m + \frac{\hbar U'''(\langle \hat{q} \rangle)^2}{32m^2\omega^5(1 + U''(\langle \hat{q} \rangle)/m\omega^2)^{5/2}}\right) \langle \ddot{\hat{q}} \rangle \\ &+ \frac{\hbar \langle \dot{\hat{q}} \rangle^2 \left(4m\omega^2 U'''(\langle \hat{q} \rangle) U''''(\langle \hat{q} \rangle)(1 + U''(\langle \hat{q} \rangle)/m\omega^2) - 5U'''(\langle \hat{q} \rangle)^3\right)}{128m^3\omega^7(1 + U''(\langle \hat{q} \rangle)/m\omega^2)^{7/2}} \\ &+ m\omega^2 \langle \hat{q} \rangle + U'(\langle \hat{q} \rangle) + \frac{\hbar U'''(\langle \hat{q} \rangle)}{4m\omega(1 + U''(\langle \hat{q} \rangle)/m\omega^2)^{1/2}} = 0. \end{split}$$

for the position expectation value. There is a new velocity-dependent contribution to the effective force at this order, and the classical mass has received a positiondependent correction. One can verify that this equation results from an action

$$\Gamma_{\rm eff}[q(t)] = \int dt \left(\frac{1}{2} \left(m + \frac{\hbar U'''(q)^2}{2^5 m^2 \left(\omega^2 + m^{-1} U''(q) \right)^{5/2}} \right) \dot{q}^2$$
(13.23)

$$-\frac{1}{2}m\omega^2 q^2 - U(q) - \frac{\hbar\omega}{2}\sqrt{1 + \frac{U''(q)}{m\omega^2}}$$
(13.24)

in agreement, to this order, with the low-energy effective action derived for instance via path integration [5]. (Although the equations of motion coincide, the meaning of q in the low-energy effective action is different from that of $\langle \hat{q} \rangle$ in canonical effective equations: q is related to off-diagonal matrix elements of \hat{q} [5] and not even guaranteed to be real. Conceptually, the low-energy effective action is thus problematic in a semiclassical context.)

13.1.6 General Properties

The examples of anharmonic systems illustrate that the solvable nature of the harmonic oscillator, not surprisingly, is very special. Solvability does not just mean that one is lucky enough to find closed solutions for a wave function. We even have closed solutions for all the moments (which would require additional integrations if derived from a wave function) and the dynamical behavior of moments of any given order is independent of the others. This strong harmonic sense of solvability is realized only rarely, in explicitly treatable but most often unrealistic ideal models. In addition to the harmonic oscillator in quantum mechanics, it can be found in the same form for free quantum field theories—or in the harmonic cosmologies of Chap. 6.

In other systems, quantum corrections arise from the back-reaction of fluctuations and higher moments. In the language of quantum field theory, these are loop corrections. The scheme presented here also produces such terms, but it is more encompassing: we obtain not only quantum-correction terms but compute state properties such as fluctuations along the way. Moments are not fixed completely, but their dynamical behavior is solved for, starting from an initial state through the initial values required to be posed for the differential equations we have. In this way, if we start with a harmonic oscillator ground state, we derive properties of the interacting ground state in the anharmonic system. For instance, from (13.21) and (13.22) we derive $(\tilde{\Delta}_0 q)^2 = \frac{1}{2} (1 + U''(\langle \hat{q} \rangle) / m\omega^2)^{-1/2}$ and $(\tilde{\Delta}_0 p)^2 = \frac{1}{2} (1 + U''(\langle \hat{q} \rangle) / m\omega^2)^{1/2}$ in the anharmonic ground state, which still saturate the uncertainty relation to the orders considered. This property is crucial for the general consistency of the scheme: At times other than the initial time, state properties are not put in from the outset, as it is sometimes suggested in other derivations based for instance on a geometrical formulation of quantum mechanics [3]. Having to prescribe the state at different times would require too much bias about the dynamical behavior especially if one evolves toward high quantum regimes.

We have also seen, for instance in the application to harmonic cosmology, that the equations shed much light on the availability and behavior of dynamical coherent states, especially in combination with the uncertainty relation. Thus, not only the interacting ground state is accessible, but a much larger class of states can be analyzed by choosing different initial values.

In comparison with the low-energy effective action we notice several new features. First, effective equations are state dependent; only when a specific state to expand around is selected, even if this is done implicitly as in most derivations of effective actions, do unique quantum-correction terms result. Not all regimes of interest clearly distinguish a unique state to expand around, such as the vacuum state, and so more freedom to parameterize state-dependent properties is present. The canonical procedure allows this freedom; for instance we may decide not to fix C_2 in the adiabatic solutions, on which only a lower bound is then given by the uncertainty relation. Secondly, general effective equations may not allow the application of an adiabatic expansion, or some other approximation in addition to the semiclassical one. In the example of anharmonic oscillators, it was the adiabaticity assumption that allowed us to solve for the moments in terms of expectation values. When there is no substitute for this assumption, moments remain a-priori undetermined and must be kept as additional independent variables. One is then dealing with a higher-dimensional effective system with true quantum degrees of freedom. This enlargement of the dimensionality is reminiscent of higher-derivative effective actions which require additional initial values to be posed for higher time derivatives of the fields. However, there is no straightforward mapping between the degrees of freedom, and in fact not all the freedom in perturbative higher-derivative effective actions is consistent [6]. The degrees of freedom of higher-dimensional canonical effective systems, on the other hand, are all consistent and have clear physical interpretations as the moments of a state.

The procedure is manageable in explicit terms if a free system is available. For canonical basic variables, this requires the Hamiltonian operator \hat{H} to be quadratic. More generally, however, there are additional options formulated by a linear system with basic operators \hat{J}_i forming a closed commutator algebra with the Hamiltonian: $[\hat{J}_i, \hat{H}] = \sum_j a_{ij} \hat{J}_j + b_i \hat{H}$. It is easy to see that such a linear algebra ensures decoupling properties of the Ehrenfest equations (13.9), which then close for the expectation values. Once a free system has been identified within a larger class of models, perturbation theory can be used to test robustness and to derive more general properties. An example for a linear system without a quadratic Hamiltonian is harmonic cosmology.

Positivity of the Hamiltonian is another important aspect. It is guaranteed for the harmonic oscillator, but it becomes an issue if systems need be reformulated to bring them in the usual Hamiltonian form, for instance by deparameterizing a constrained system. Especially if the system is relativistic, a square root must be taken and combined with a judicious sign choice. We may for instance have a constraint of the form $p_{\varphi}^2 - H^2 = 0$ as in relativistic deparameterizable systems (Sect. 12.3.2). Taking a square root $p_{\varphi} = \pm |H|$ means that the absolute value may destroy strict linearity, as already discussed in the context of cosmology. As we will see in more detail in the next section, quantum constraints can be dealt with just like quantum Hamiltonians, by taking the expectation value as a function on the state space and expanding in the moments. There are several differences compared to a non-relativistic system; for instance, additional moments of p_{φ} may contribute to quantum constraints unlike in the linearized deparameterized version. For now, we are interested only in the fact that we will have to take a square root when solving for p_{φ} and bringing the system to deparameterized form.

A sign ambiguity thus arises in solving for $p_{\varphi} = \pm |H|$ to obtain the two sectors of positive-frequency and negative-frequency modes. No difference occurs between classical and effective constraints from this perspective. But the nature of a linear quantum system may be spoiled by the absolute value around H. Even if H is quadratic in canonical variables, such as H = cp in the solvable model of Wheeler– DeWitt cosmology, |H| is not strictly quadratic. However, on states supported only on the positive or negative part of the spectrum of H, respectively, the absolute value can be dropped and the system will be linear. If H is time-independent, the required spectral property of states will be preserved and it is necessary to restrict only initial values to the spectral property. This can easily be done without too strong restrictions on the moments and the accessible states.

In a Hilbert-space representation, $|\hat{cp}|$ is usually a non-local operator if wave functions such as $\psi(c)$ or $\psi(p)$ are used. However, this kind of non-locality is representation dependent (and thus unphysical). An operator of this form would

certainly be local in a representation based on eigenstates of the operator \hat{cp} . Since effective equations are representation-independent, they are insensitive to this non-locality problem.

13.2 Effective Constraints

As already indicated, a constraint operator gives rise to the quantum constraint $C_Q = \langle \hat{C} \rangle = C_{\text{class}}(q, p) + \cdots$ on the state space since it must vanish when the expectation value is taken in physical states. Quantum corrections to the classical constraint surface thus arise. However, a single constraint on the quantum phase space only removes two degrees of freedom (by constraining and factoring out a gauge, provided the constraint is part of a first-class system). Corresponding quantum variables would remain unconstrained, leaving infinitely many spurious variables which would never arise in a quantization of the classical reduced phase space.

Removing all degrees of freedem as appropriate requires additional constraints. In fact, there are infinitely many ones

$$C_{f(q,p)} := \langle f(\hat{q}, \hat{p}) \hat{C} \rangle$$

on the state space, which all have to vanish in physical states and which in general are independent of C_Q . Practically, one can usually work with polynomials f(q, p), as we will also see in examples below. As with the truncations in the discussion of effective dynamics, solutions of the constraints become feasible to any given order in moments, where only finitely many C_f have to be considered.

At this general level, several properties important for the consistency of the constrained system can be derived [7]. The system of constraints is first-class if the ordering $\langle f(\hat{q}, \hat{p})\hat{C}\rangle$ is indeed used as indicated in the definition. This means that we are dealing with operator products not symmetric in general. Naive reorderings either spoil the first-class nature, or lead to functions that are not constraints if the constraint operator no longer stands at the very right or left of the operator product. Alternatively, one may define quantum constraints via the generating functional $C_{\alpha} = \langle e^{i\hbar^{-1}\alpha_i \cdot \hat{x}^i} C(\hat{x}^i) \rangle$ (where $(\hat{x}^i)_{i=1,2} = (\hat{q}, \hat{p})$) for Weyl-ordered and thus symmetric constraints, which also provides a first-class system. This procedure does include certain reorderings of our constraints above, obtained by all possible derivatives of C_{α} by the components α_i , and then setting $\alpha = 0$. But practically it is not always easy to derive the Weyl-ordered constraints and we will continue with the non-symmetric constraints.

In fact, we do not require reality of kinematical quantum variables $\Delta(q^a p^b)$, realized before constraints are solved. Usually the kinematical inner product has to be changed to the physical one after the constraints are solved, and requiring self-adjointness or reality before this step would not guarantee the correct reality properties. Then there is no reason either to require constraint functions to be real, or to come from symmetrically ordered operator products including the constraint. We

will impose reality conditions only after solving the constraints to ensure physical normalization. In this way, physical observables are accessible without deriving the full physical Hilbert space or a specific integral form of the physical inner product. Also here, the procedure is very well amenable to perturbative techniques, which is not the case for other constructions of physical Hilbert spaces.

Different gauge fixings of the constrained system can in some cases be seen to be related to different kinematical Hilbert space structures. Results will thus be independent of ambiguities that otherwise arise by choosing a particular kinematical Hilbert space as one does in group averaging. Moreover, since Hilbert-space representations are not referred to, no difference in the treatment arises between constraints with zero in their discrete or continuous spectra.

13.2.1 Non-Relativistic Constraints

Non-relativistic constraints are characterized by a linear dependence on one momentum variable which can be considered as an energy. In non-relativistic deparameterizable systems, this linear momentum is conjugate to a global time variable. From the point of view of physical Hilbert spaces as well as effective constraints this case is easier to deal with, and we discuss it first by way of examples.

Example 13.6 (*Linear constraint*) Let us take a constraint $\hat{C} = \hat{p}$. It immediately implies $\langle \hat{p} \rangle = 0$, while $\langle \hat{q} \rangle$ is pure gauge. At second order of the moments, we have $(\Delta p)^2 = 0$ fully constrained, while $C_q = \langle \hat{q} \hat{p} \rangle = 0$ implies the complex-valued kinematical covariance

$$\Delta(qp) = \frac{1}{2} \langle \hat{q} \, \hat{p} + \hat{p} \hat{q} \rangle - \langle \hat{q} \rangle \langle \hat{p} \rangle = -\frac{1}{2} \mathrm{i}\hbar.$$

At least one of the kinematical variables must thus take complex values, which means that we indeed have to redefine our kinematical inner product for the physical Hilbert space. Dealing with complex variables cannot always be avoided; it even has an advantage: the uncertainty relation

$$(\Delta q)^2 (\Delta p)^2 - \Delta (qp)^2 \ge \frac{1}{4}\hbar^2$$

remains respected even though one of the fluctuations, Δp , vanishes. (The other one, Δq , is pure gauge.) With the uncertainty relation at one's disposal, one can analyze dynamical coherent states also for constrained systems.

Example 13.7 (Two-component linearly constrained system and physical observables [7]) We now assume a constraint $\hat{C} = \hat{p}_1 - \hat{p}$ which is still linear but defined for a system with two independent pairs of degrees of freedom. We denote the kinematical quantum variables as

$$\Delta(p^a q^b p_1^c q_1^d) = \langle (\hat{p} - p)^a (\hat{q} - q)^b (\hat{p}_1 - p_1)^c (\hat{q}_1 - q_1)^d \rangle_{\text{symm}}.$$

As second-order constraints in addition to $C_Q = \langle \hat{p}_1 \rangle - \langle \hat{p} \rangle$ we have

$$C_{q} = -\frac{i\hbar}{2} - \Delta(qp) + \Delta(qp_{1}), \quad C_{p} = \Delta(pp_{1}) - (\Delta p)^{2}$$
$$C_{p_{1}} = (\Delta p_{1})^{2} - \Delta(pp_{1}), \quad C_{q_{1}} = \frac{1}{2}i\hbar - \Delta(pq_{1}) + \Delta(q_{1}p_{1})$$

solved by $\langle \hat{p}_1 \rangle = \langle \hat{p} \rangle$ and

$$\Delta(qp_1) \approx \frac{1}{2}i\hbar + \Delta(qp), \quad \Delta(pp_1) \approx (\Delta p)^2$$
$$(\Delta p_1)^2 \approx \Delta(pp_1) \approx (\Delta p)^2, \quad \Delta(pq_1) \approx \frac{1}{2}i\hbar + \Delta(q_1p_1).$$

To derive observables, we also need the gauge flows which, for instance for C_p , are of the form

$$\begin{split} \delta\Delta(qp) &= \Delta(pp_1) - 2(\Delta p)^2 \approx -(\Delta p)^2 \\ \delta(\Delta q)^2 &= 2\Delta(qp_1) - 4\Delta(qp) \approx i\hbar - 2\Delta(qp) \\ \delta\Delta(q_1p_1) &= \Delta(pp_1) \approx (\Delta p)^2 \\ \delta\Delta(qq_1) &= \Delta(q_1p_1) + \Delta(qp) - 2\Delta(pq_1) \approx \Delta(qp) - \Delta(q_1p_1) - i\hbar \\ \delta(\Delta q_1)^2 &= \Delta(pq_1) \approx i\hbar + 2\Delta(q_1p_1). \end{split}$$

It is easy to check that all gauge flows satisfy $\delta \Delta(qp) = -\delta \Delta(q_1p_1)$, $\delta \Delta(qq_1) = -\frac{1}{2} \left(\delta(\Delta q)^2 + \delta(\Delta q_1)^2 \right)$. Thus, the functions

$$(\mathscr{D}q)^{2} := (\Delta q)^{2} + 2\Delta(qq_{1}) + (\Delta q_{1})^{2}$$
(13.25)

$$(\mathscr{D}p)^2 := (\Delta p)^2 \tag{13.26}$$

$$\mathscr{D}(qp) := \Delta(qp) + \Delta(q_1p_1) + \frac{1}{2}i\hbar$$
(13.27)

on the kinematical state space are gauge invariant. They also satisfy the correct algebra

$$\{(\mathscr{D}q)^2, \mathscr{D}(qp)\} = 2(\mathscr{D}q)^2 \tag{13.28}$$

$$\{(\mathscr{D}q)^2, (\mathscr{D}p)^2\} = 4\mathscr{D}(qp) \tag{13.29}$$

$$\{(\mathscr{D}(qp), (\mathscr{D}p)^2\} = 2(\mathscr{D}p)^2$$
(13.30)

expected for second-order quantum variables on a reduced state space. For this, the imaginary contribution in (13.27) is required, which need not be added just to make $\mathscr{D}(qp)$ gauge-invariant. At this stage, all moments involving the pair (q_1, p_1) are

either expressed in terms of (q, p)-moments by solving constraints, or subject to gauge. (One could certainly as well choose to express the (q, p)-moments in terms of the (q_1, p_1) ones.)

We finally impose reality conditions: $\mathscr{D}(q^a p^b) \in \mathbb{R}$. The observable moments can then be seen as those computed in a physical Hilbert space. Expressed in terms of kinematical quantum variables, this again requires an imaginary part $\operatorname{Im}(\Delta(qp) + \Delta(q_1p_1)) = -\frac{1}{2}i\hbar$ for $\mathscr{D}(qp) := \Delta(qp) + \Delta(q_1p_1) + \frac{1}{2}i\hbar$ to be real. Since kinematical quantum variables must be complex to provide correct physical reality (although they appear symmetrically ordered), we have an explicit example in which the kinematical Hilbert-space structure must be changed when deriving the physical Hilbert space. We can also see explicitly that different kinematical choices are possible, such as $\Delta(qp)$ real or $\Delta(q_1p_1)$ real. They imply different kinematical reality conditions, all resulting in the same physical observables, and thus correspond to different kinematical Hilbert space structures.

This simple example can be used to illustrate one aspect of the problem of time and how it can be overcome by effective techniques; see also Sect. 13.2.3. In the preceding example we could easily choose q as time instead of q_1 ; the choice is simply a question of gauge fixing of the effective constraints. If one were to implement the constraints for physical states in a Hilbert space, on the other hand, the situation would be more subtle. The constraint equations could certainly still be solved easily, and physical inner products be constructed, for instance by group averaging. However, the different choices of time are difficult to compare at the Hilbert-space level, where no obvious mapping between the two deparameterized Hilbert spaces exists. In this simple model one could easily postulate a natural mapping thanks to the symmetric way in which q and q_1 and their momenta appear. For general constraints still provide comparisons between different choices of time via the corresponding gauge fixings.

Explicit derivations as in the case of a linear constraint are more complicated when constraints are non-linear since different orders of moments are mixed in expectation values. But similar structures for solutions to constraints and observables remain realized.

Example 13.8 (*Free particle*) A parameterized free particle has the constraint $\hat{C} = \hat{p}_t + \hat{p}^2/2M$, and thus $C_Q = \langle \hat{p}_t \rangle + \langle \hat{p} \rangle^2/2M + (\Delta p)^2/2M$, $C_q = \Delta(qp_t) + i\hbar \langle \hat{p} \rangle/2M + \langle \hat{p} \rangle \Delta(qp)/M$ and so on [7]. Solving the constraints is more involved than in the linear case, but the procedure is the same. Now, second-order observables are $\mathscr{P} = \langle \hat{p} \rangle$, $\mathscr{Q} = \langle \hat{q} \rangle - \langle \hat{t} \rangle \langle \hat{p} \rangle/M - \Delta(pt)/M$ and

$$(\mathcal{D}p)^2 = (\Delta p)^2$$
$$\mathcal{D}(qp) = \Delta(qp) + \Delta(tp_t) - \frac{\langle \hat{t} \rangle}{M} (\Delta p)^2 + \frac{i\hbar}{2}$$

$$= (\Delta q)^2 - 2\frac{\langle \hat{p} \rangle}{M} \Delta(qt) + \frac{\langle \hat{p} \rangle^2}{M^2} (\Delta t)^2 - \frac{2\langle \hat{t} \rangle}{M} \left(\Delta(qp) + \Delta(tp_t) + \frac{i\hbar}{2} \right) + \frac{\langle \hat{t} \rangle^2}{M^2} (\Delta p)^2$$

with explicit couplings between kinematical expectation values and moments. Also here, second-order moments satisfy the correct algebra. For a free particle, we do not expect quantum back-reaction in the kinematical quantities, even though physical expectation values depend on some moments. The relationship can be understood by deparameterizing: We invert our equations for the observables to obtain

$$\begin{split} \langle \hat{q} \rangle (\langle \hat{t} \rangle) &= \mathcal{Q} + \frac{\langle \hat{t} \rangle}{M} \mathcal{P} + \frac{1}{M} \Delta(pt) \\ &\approx \mathcal{Q} + \frac{\langle \hat{t} \rangle}{M} \mathcal{P} - \frac{1}{\langle \hat{p} \rangle} \left(\Delta(tp_t) + \frac{i\hbar}{2} \right) \\ &= \mathcal{Q} + \frac{\langle \hat{t} \rangle}{M} \mathcal{P} - \frac{1}{\mathcal{P}} \left(\mathcal{Q}(qp) + \frac{\langle \hat{t} \rangle}{M} (\mathcal{Q}p)^2 - \Delta(qp) \right) \end{split}$$

and now interpret the observable coefficients as integration constants. For the gauge choice $\Delta(tp_t) = -\frac{1}{2}i\hbar$ identical to what we used before, we have correct deparameterized solutions

$$\langle \hat{q} \rangle (\langle \hat{t} \rangle) = \mathscr{Q} + \frac{\langle \hat{t} \rangle}{M} \mathscr{P}, \quad \Delta(qp)(\langle \hat{t} \rangle) = \mathscr{Q}(qp) + \frac{\langle \hat{t} \rangle}{M} (\mathscr{Q}p)^2$$
(13.31)

in terms of initial values. These equations can also be interpreted as relational observables between the remaining degree of freedom and time. (The gauge choice used is not unique, but is the only one good for all \mathscr{P} . Moreover, it implies real $\Delta(qp)$, but imaginary $\Delta(tp_t)$ as it is realized in the deparameterized, time-independent kinematical Hilbert space. This gauge choice is the one corresponding to the usual Schrödinger representation of the deparameterized system, whose solutions for $\langle \hat{q} \rangle(t)$ and $\Delta(qp)(t)$ are the same as (13.31). Other gauge choices provide different deparameterized relationships, and are more difficult to formulate in a Hilbert-space setting.)

The presence of quantum variables such as the covariance opens up new possibilities for internal times and deparameterization, compared to a classical system. In fact, the squeezing of a state has often been brought in contact with entropy and the second law of thermodynamics, implying monotonic behavior [8–14]. Thus, a quantum variable such as $\Delta(qp)$ may provide a good internal time even in regions where all classical variables would behave in an oscillatory manner [15, 16]. It would also imply that a natural concept of time would in fact include a strong quantum component, showing a possible quantum origin of time.

13.2.2 Relativistic Systems

Relativistic systems can be treated in much the same way as non-relativistic ones. A major advantage of effective techniques in this context is the fact that square roots need not be taken at the operator level (for which one would have to know the complete spectral decomposition of the Hamiltonian) but simply for numbers such as expectation values. We demonstrate these features using the previous Example 12.5 of the relativistic harmonic oscillator [17]. Up to second order in moments, the effective constraints are

$$C = \langle \hat{p}_{\varphi} \rangle^2 - \langle \hat{p} \rangle^2 - \langle \hat{q} \rangle^2 + (\Delta p_{\varphi})^2 - (\Delta p)^2 - (\Delta q)^2$$
(13.32)

$$C_{\varphi} = 2\langle \hat{p}_{\varphi} \rangle \Delta(\varphi p_{\varphi}) + i\hbar \langle \hat{p}_{\varphi} \rangle - 2\langle \hat{p} \rangle \Delta(\varphi p) - 2\langle \hat{q} \rangle \Delta(\varphi q)$$
(13.33)

$$C_{p_{\varphi}} = 2\langle \hat{p}_{\varphi} \rangle (\Delta p_{\varphi})^2 - 2\langle \hat{p} \rangle \Delta(p_{\varphi}p) - 2\langle \hat{q} \rangle \Delta(p_{\varphi}q)$$
(13.34)

$$C_q = 2\langle \hat{p}_{\varphi} \rangle \Delta(p_{\varphi}q) - 2\langle \hat{p} \rangle \Delta(qp) - i\hbar \langle \hat{p} \rangle - 2\langle \hat{q} \rangle (\Delta q)^2$$
(13.35)

$$C_p = 2\langle \hat{p}_{\varphi} \rangle \Delta(p_{\varphi}p) - 2\langle \hat{p} \rangle (\Delta p)^2 - 2\langle \hat{q} \rangle \Delta(qp) + i\hbar \langle \hat{q} \rangle.$$
(13.36)

Thus, some kinematical moments must be complex. Going through the solution procedure for first-class constraints applied to this system [18], solving (13.32) for $\langle \hat{p}_{\varphi} \rangle$ and eliminating all p_{φ} - and φ -moments using the other effective constraints, one can see that the system is deparameterizable in φ with quantum Hamiltonian $\langle \hat{p}_{\varphi} \rangle = \pm H_Q$,

$$H_{Q} = \sqrt{\langle \hat{p} \rangle^{2} + \langle \hat{q} \rangle^{2}} \left(1 + \frac{\langle \hat{q} \rangle^{2} (\Delta p)^{2} - 2 \langle \hat{q} \rangle \langle \hat{p} \rangle \Delta (qp) + \langle \hat{p} \rangle^{2} (\Delta q)^{2}}{2 (\langle \hat{p} \rangle^{2} + \langle \hat{q} \rangle^{2})^{2}} \right).$$

Reality is then imposed on Dirac observables $\langle \hat{q} \rangle (\langle \hat{\varphi} \rangle), \langle \hat{p} \rangle (\langle \hat{\varphi} \rangle), \Delta(\cdots) (\langle \hat{\varphi} \rangle)$ obtained by solving the Hamiltonian equations.

13.2.3 Problem of Time

Dirac observables of the effective constrained system provide the observable information just as one could compute it on the physical Hilbert space when a particular representation is known. But now, in addition to the difficult task of computing a complete set of obervables for the reduced phase space, we have a second option which does not have an analog at the Hilbert-space level: we can treat the constrained system by gauge fixing. An analysis of the constraints and the gauge flow they generate shows that one can fix the gauge (to second order in moments) by requiring the moments $(\Delta \varphi)^2$, $\Delta(\varphi q)$ and $\Delta(\varphi p)$ to vanish when one decides to use $\langle \hat{\varphi} \rangle$ as time. Other moments involving time are then fixed by solving the constraints, such that no φ -moments remain free. This outcome is just as expected if one were to choose φ as time from the outset and then quantize the system with φ as a parameter, not an operator. Now, however, the procedure easily allows the use of $\langle \hat{\varphi} \rangle$ as a local internal time: one may use different gauge fixings to describe different parts of the phase space, and one may easily transfer to a different choice of time by applying a gauge transformation. Following [19], the gauge fixing that implements a specific choice of time is called a Zeitgeist.

Once a Zeitgeist is specified, we gain access to properties of $\langle \hat{\varphi} \rangle$, which are interesting in the context of time even though this parameter is not an observable on the reduced phase space. In particular, the value changes when a different time is used; it depends on the Zeitgeist. As the following example illustrates, a general consequence is that time is complex.

Example 13.9 (*Time-dependent potential*) We consider a constraint operator $\hat{C} = \hat{p}_{\varphi}^2 - \hat{p}^2 + V(\hat{\varphi})$ for a relativistic particle in an arbitrary φ -dependent potential $V(\varphi)$. The notation indicates that we are going to choose φ as internal time, but this choice is not required from the outset. In particular, φ may not serve as global internal time classically; there may be turning points where p_{φ} vanishes and φ fails to be a well-defined parameter along solutions. The constraint operator gives rise to the effective constraints

$$C_Q = \langle \hat{p}_{\varphi} \rangle^2 - \langle \hat{p} \rangle^2 + (\Delta p_{\varphi})^2 - (\Delta p)^2 + V(\langle \hat{\varphi} \rangle) + \frac{1}{2} V''(\langle \hat{\varphi} \rangle) (\Delta \varphi)^2 \quad (13.37)$$

$$C_{\varphi} = 2\langle \hat{p}_{\varphi} \rangle \Delta(\varphi p_{\varphi}) + i\hbar \langle \hat{p}_{\varphi} \rangle - 2p\Delta(\varphi p) + V'(\langle \hat{\varphi} \rangle)(\Delta \varphi)^2$$
(13.38)

$$C_{p_{\varphi}} = 2\langle \hat{p}_{\varphi} \rangle (\Delta p_{\varphi})^{2} - 2\langle \hat{p} \rangle \Delta(p_{\varphi}p) + V'(\langle \hat{\varphi} \rangle) \left(\Delta(\varphi p_{\varphi}) - \frac{1}{2} \mathrm{i}\hbar \right)$$
(13.39)

to second order in the moments. We now implement $\langle \hat{\varphi} \rangle$ as local internal time via the Zeitgeist

$$(\Delta \varphi)^2 = \Delta(\varphi q) = \Delta(\varphi p) = 0.$$
(13.40)

We see that $\Delta(\varphi p_{\varphi}) = -\frac{1}{2}i\hbar$ from $C_{\varphi} = 0$, which then implies

$$(\Delta p_{\varphi})^{2} = \frac{\langle \hat{p} \rangle^{2}}{\langle \hat{p}_{\varphi} \rangle^{2}} (\Delta p)^{2} + \frac{1}{2} i \frac{V'(\langle \hat{\varphi} \rangle)\hbar}{\langle \hat{p}_{\varphi} \rangle}$$

because of $C_{p_{\omega}} = 0$. With this, we arrive at the expression

$$C = \langle \hat{p}_{\varphi} \rangle^{2} - \langle \hat{p} \rangle^{2} + \frac{\langle \hat{p} \rangle^{2} - \langle \hat{p}_{\varphi} \rangle^{2}}{\langle \hat{p}_{\varphi} \rangle^{2}} (\Delta p)^{2} + \frac{1}{2} i \frac{V'(\langle \hat{\varphi} \rangle)\hbar}{\langle \hat{p}_{\varphi} \rangle} + V(\langle \hat{\varphi} \rangle)$$
(13.41)

for the constraint $C_Q = \langle \hat{C} \rangle$ on the space on which C_{φ} and $C_{p_{\varphi}}$ are solved.

In (13.41), all terms except the last two are expected to be real-valued: $\langle \hat{p} \rangle$ and Δp are physical observables for the class of systems considered, and $\langle \hat{p}_{\varphi} \rangle$ can be

interpreted physically as the local energy value. When the constraint is satisfied, we obtain the imaginary part of $\langle \hat{\varphi} \rangle$ from

$$\frac{1}{2}i\frac{V'(\langle\hat{\varphi}\rangle)\hbar}{\langle\hat{p}_{\varphi}\rangle} + V(\langle\hat{\varphi}\rangle) = 0.$$
(13.42)

For semiclassical states, to which this approximation of effective constraints refers, we Taylor expand the potential

$$V(\langle \hat{\varphi} \rangle) = V(\operatorname{Re}\langle \hat{\varphi} \rangle + i\operatorname{Im}\langle \hat{\varphi} \rangle) = V(\operatorname{Re}\langle \hat{\varphi} \rangle) + i\operatorname{Im}\langle \hat{\varphi} \rangle V'(\operatorname{Re}\langle \hat{\varphi} \rangle) + O((\operatorname{Im}\langle \hat{\varphi} \rangle)^2)$$

in the imaginary term, expected to be of the order \hbar . To order \hbar , the imaginary contribution to *C* is given by

$$\frac{1}{2}i\frac{V'(\operatorname{Re}\langle\hat{\varphi}\rangle)\hbar}{\langle\hat{p}_{\varphi}\rangle} + iV'(\operatorname{Re}\langle\hat{\varphi}\rangle)\operatorname{Im}\langle\hat{\varphi}\rangle + O(\hbar^{3/2}) = 0.$$

Thus,

$$\operatorname{Im}\langle\hat{\varphi}\rangle = -\frac{\hbar}{2\langle\hat{p}_{\varphi}\rangle}.$$
(13.43)

As a consistency result, one can check that changing the Zeitgeist by a gauge transformation transfers the imaginary contribution from $\langle \hat{\varphi} \rangle$ to the new variable used as local internal time [20].

At this stage, one may note that the possibility of time as an operator has often been considered in quantum mechanics, with the conclusion that it could not be selfadjoint. Otherwise, it would generate unitary transformations changing the energy by arbitrary amounts, in conflict with the expectation that energy should be bounded from below for stability. A non-self-adjoint time operator would not be guaranteed to have a real-valued expectation value, a consequence which seems in agreement with what we have found here in explicit form. However, the result (13.43) is of a more general nature: it applies whenever there is a time-dependent potential, irrespective of whether it has a lower bound. Even if the potential is bounded neither from above nor from below do our results hold, but arguments using the energy-translation generated by time would no longer apply to tell us whether time could be real.

13.3 Applications of Effective Constraints in Quantum Gravity and Cosmology

Canonical quantum gravity is plagued by several long-standing problems which have not been resolved so far. While loop quantum gravity has introduced many new ingredients in this field, it has barely been able to touch these difficult issues. Central among them are the problem of time [21] and the anomaly problem, and they must

both be solved before a consistent framework to derive physical predictions can be obtained. Effective-constraint techniques allow one to address these problems in a new way, and to solve them in semiclassical regimes where effective constraints can be truncated and analyzed. This procedure does not eliminate the problems altogether, but it considerably tames them for most practical purposes.

13.3.1 Problem of Time

The effective procedure to deal with non-deparameterizable constraints has several advantages. Regarding the problem of time, local internal times and local relational observables can be consistently implemented in quantum systems [19, 20]. Changing the internal time simply amounts to a gauge transformation; the equivalence of different choices of time easily follows. As illustrated for instance by the fact that the imaginary part of time is transferred when the time is changed, the procedure is consistent. In particular, one can require that all physical observables be real even in the presence of complex time. In fact, the complexity of time is crucial for the consistency of the whole framework; requiring time expectation values to be real would lead to contradictions with physical reality conditions. Complex time is thus an important part of a consistent procedure to solve quantum constrained systems.

13.3.2 Anomaly Problem

Effective constraints are also useful to analyze the anomaly problem, as we have already done for perturbation equations subject to inverse-triad corrections. For an anomaly-free quantization of several constraints \hat{C}_I , effective constraints $C_{f,I} = \langle f(\hat{q}, \hat{p})\hat{C}_I \rangle$ satisfy a first-class system. But it is not always easy to quantize in an anomaly-free way, such that constraint operators of a classical first-class system would indeed be first-class. The first-class nature required for this is rather strong since it is off-shell: it must be realized even off the solution space of the constraints since anomaly-freedom would have to be checked before solving the constraints. (The importance of properties of the off-shell algebra has been emphasized in [22].)

Effective techniques allow more direct ways of implementing anomaly-freedom: One first formulates effective constraints for a possible quantization parameterized by different choices (such as factor ordering or other ambiguities). At this stage no inconsistency arises even if the corresponding constraint operators are not anomalyfree; inconsistencies would result only when one tries to solve the constraints. Before doing so, one can compute the Poisson algebra of the effective constraints and check under which conditions, or if at all, it can be first-class. As always, this can be done order by order and is much more feasible than a calculation of the full algebra of operators. If an anomaly-free version exists, one can pick this first-class version of effective constraints for further calculations. This is the procedure we followed in Sect. 10.3 for inverse-triad corrections in loop quantum gravity.

All this is more tractable than full quantum commutators, and yet it provides consistent constraints incorporating quantum corrections. As a side product, it shows how strongly kinematical quantization ambiguities are reduced by dynamical consistency.

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