Chapter 2
Observables, Symmetries and Constraints

Abstract The notion of observable is one of the key concepts of a physical theory. We introduce a definition of observables within the framework of ensembles on configuration space, based on the idea of associating observables with generators of canonical transformations acting on the phase space of the fundamental variables P and S. These ensemble observables encompass both classical and quantum observables. Remarkably, for classical observables the Poisson bracket of the ensemble observables is isomorphic to the usual bracket on standard classical phase space, while for quantum observables it is isomorphic to the commutator in Hilbert space. We show that the formalism allows for the generalisation of certain quantum concepts, such as eigenstates, eigenvalues, weak values and transition probabilities, to arbitrary configuration ensembles. We discuss also systems with symmetries, in particular examples which involve representations of the Galilean group for the case of a free particle and rotations defined on discrete configuration spaces. Finally, we generalise and reinterpret quantum superselection rules in terms of constraints on observables.

2.1 Some General Considerations

The description of physical systems in terms of ensembles on configuration space introduces very few physical assumptions. However, there are some issues which concern the *interpretation* of the basic elements that are part of the formalism which are of importance and which we now address.

2.1.1 Fundamental Variables and Ontology

The theory of ensembles on configuration space is a statistical theory which describes states of a system (classical, quantum or hybrid) in terms of the two canonically conjugate variables, P and S, with the time evolution of the conjugate variables being determined by an ensemble Hamiltonian, $\mathscr{H}[P, S]$ (see Chap. 1).

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The interpretation of P is rather straightforward. We assume that the configuration of a physical system is an inherently statistical concept, in which case the state of the system must be described by an ensemble of configurations, corresponding to some probability density P on the configuration space. The physical interpretation of S requires more care. As we have discussed in the previous chapter, the dynamical significance of S is invariant under addition of an arbitrary constant, and one may define a local energy density, $-P\partial_t S$, for ensemble Hamiltonians satisfying a fundamental homogeneity property. Furthermore, the gradient of S plays an important role for continuous configuration spaces because it is proportional to the velocity vector fields which enters into the continuity equation for P (see Sect. 1.2), and its more general role as a generator of translations will be seen below. It is clear that one could attempt to "complete" the theory, for example by assigning a definite momentum $\mathbf{p} = \nabla S$ and a definite energy $E = -\partial_t S$ to particles that belong to an ensemble. This would lead to the usual deterministic interpretation of the Hamilton–Jacobi equation for the case of a classical system, and to the de Broglie–Bohm formulation for the case of a quantum system. However, we will not take this additional step and we will rely instead on a "minimalist" interpretation in which the theory is treated as a purely *statistical* one (see also the discussion of the classical limit in Sect. 9.3). Thus, for particles and continuous configuration spaces, the fundamental concept is that of a probability density P defined on the configuration space of the system, and the existence of a canonically conjugate quantity S is mandated by the requirement that P evolves according to an action principle.

A configuration ensemble defined by a pair of conjugate variables P and S which satisfy the equations of motion derived from the ensemble Hamiltonian will also be called a *pure ensemble*. This terminology corresponds to the notion of a pure state in quantum mechanics, which is described by a wave function $\psi = \sqrt{P}\mathrm{e}^{\mathrm{i}S/\hbar}$ (in contrast to a mixed state described by a density matrix). Here we apply this terminology to all configuration ensembles, whether classical, quantum or otherwise. In addition, one may also define *mixtures* of configuration ensembles, of the form $\{P_k, S_k; w_k\}$, where each of the components satisfy the equations of motion determined by the same ensemble Hamiltonian $\mathscr{H}[P, S]$ and $\sum_k w_k = 1$, so that $\sum_k w_k \int \mathrm{d}x\, P_k(x, t) = 1$. Mixtures are integral to our discussion of thermodynamics on configuration space in Chap. 4. But the formalism of ensembles on configuration space has a *pure state ontology*. In particular, it treats pure ensembles, rather than more general mixtures, as physically fundamental. The latter are taken to merely reflect ignorance of the 'true' pure state.

2.1.2 The Dual Role of Observables

From quantum mechanics, we are familiar with the dual role of the operators that are associated with observables: they are Hermitian operators which, on the one hand, generate transformations which are unitary and thus preserve the normalization of the probability $|\psi|^2$ and, on the other, have real expectation values and eigenvalues which in principle can be determined from measurement (hence the terminology "observable"). It is often necessary to consider *both* roles when analyzing experiments: typically, an effort is made to prescribe operational procedures which define the observables that are being measured in the experiment via a particular interaction process (e.g., the spin of a particle in a Stern–Gerlach experiment via an interaction with an inhomogeneous magnetic field) while at the same time including other observables in the analysis of the experiment in their role of generators of transformations (e.g., the energy in its role of generator of time translations, if the interaction takes place at one time and the detection at a later time).

As is well known, for most of the Hermitian operators that one can define in quantum mechanics there are no operational procedures that specify how they should be measured. In addition, there are fundamental limitations on the precision with which measurements can be made for observables that do not commute with additive conserved quantities (e.g., linear or angular momentum, or charge) [1], which constitute however the vast majority of the observables that are of interest. This does not create serious difficulties when applying quantum theory to actual experiments, but it does mean that the theory allows for a surplus of possible observables, all of which have well defined properties as far as their role as generators of transformations is concerned, but are problematic in their role of measurable quantities in that operational prescriptions for eigenvalues and expectation values are not always available.

A similar situation, regarding both the dual role of observables and the large number of possible observables allowed by the theory, also holds for standard classical dynamics on phase space: observables are functions of position and momentum on phase space, and are regarded as both measurable quantities and generators of canonical transformations [2].

In the discussion on observables that follows, for the general case of ensembles on configuration space, the same considerations apply. We will first address the more general issue of defining generators of transformations within the theory. We will make the connection to measurements in Chap. 3.

In this chapter we give a precise definition of observables, and discuss examples for both classical and quantum ensembles. We introduce the notion of an eigenensemble, and generalise the quantum mechanical notions of weak values and transition probabilities. We address the representation of symmetries by corresponding groups of observables, independently of whether the ensemble is classical, quantum or otherwise, via examples of Galilean particles and "rotational bits". Finally, we end the Chapter with a discussion of constraints and the formulation of superselection rules.

2.2 Observables

A significant advantage of describing physical systems by ensembles evolving on configuration space is the existence of an action principle (see Chap. 1). In particular, this allows the definition of a Poisson bracket for functions of the fundamental phase space variables P and S, and allows observables to be introduced as generators of canonical transformations with respect to this bracket, just as in standard classical dynamics [2]. We will see that this Poisson bracket is isomorphic to the Poisson bracket on a classical phase space for the case of classical ensembles, and is isomorphic to the quantum commutator for the case of quantum observables. The existence of such a bracket will more generally allow us to define dynamics for hybrid classical-quantum systems, such as the coupling of quantum systems to classical measuring apparatuses and of quantum fields to classical gravity (see Chaps. 8 and 11).

For an ensemble on a discrete configuration space, with ensemble Hamiltonian $\mathscr{H}(P, S)$, the evolution is specified by the Hamiltonian equations of motion (see Chap. 1)

$$\frac{\partial P_j}{\partial t} = \frac{\partial H}{\partial S_j}, \quad \frac{\partial S_j}{\partial t} = -\frac{\partial H}{\partial P_j}. \tag{2.1}$$

Defining the Poisson bracket for two arbitrary functions $A(P, S)$ and $B(P, S)$ by

$$\{A, B\} := \sum_j \left(\frac{\partial A}{\partial P_j}\frac{\partial B}{\partial S_j} - \frac{\partial A}{\partial S_j}\frac{\partial B}{\partial P_j} \right), \tag{2.2}$$

these equations of motion may be rewritten in the form

$$\frac{\partial P_j}{\partial t} = \{P_j, \mathscr{H}\}, \quad \frac{\partial S_j}{\partial t} = \{S_j, \mathscr{H}\} \tag{2.3}$$

in complete analogy to the case of classical phase space dynamics [2]. It immediately follows that any function $A(P, S, t)$ of P, S and t evolves as

$$\begin{aligned} \frac{\mathrm{d}A}{\mathrm{d}t} &= \sum_j \left(\frac{\partial A}{\partial P_j}\frac{\partial P_j}{\partial t} + \frac{\partial A}{\partial S_j}\frac{\partial S_j}{\partial t} \right) + \frac{\partial A}{\partial t} \\ &= \{A, \mathscr{H}\} + \frac{\partial A}{\partial t}. \end{aligned} \tag{2.4}$$

Similarly, for an ensemble on a continuous configuration space, the Poisson bracket of two arbitrary functionals $A[P, S]$ is defined by

$$\{A, B\} = \int \mathrm{d}x \left(\frac{\delta A}{\delta P}\frac{\delta B}{\delta S} - \frac{\delta A}{\delta S}\frac{\delta B}{\delta P} \right). \tag{2.5}$$

Noting that $\delta f(x)/\delta f(x') = \delta(x - x')$ (see Appendix A.1 of this book), it follows that the equations of motion for the ensemble can be rewritten as

$$\frac{\partial P}{\partial t} = \{P, \mathscr{H}\}, \quad \frac{\partial S}{\partial t} = \{S, \mathscr{H}\} \tag{2.6}$$

and that again $\mathrm{d}A/\mathrm{d}t = \{A, \mathscr{H}\} + \partial A/\partial t$ as per Eq. (2.4).

Transformations of the fundamental phase space variables P and S that preserve the Poisson bracket are called canonical transformations. In particular, every function (or functional) of these variables generates an associated infinitesimal canonical transformation, according to

$$\delta P = \{P, A\}\varepsilon = \frac{\delta A}{\delta S}\varepsilon \tag{2.7}$$

$$\delta S = \{S, A\}\varepsilon = -\frac{\delta A}{\delta P}\varepsilon, \tag{2.8}$$

where ε is an infinitesimal parameter [2].

It is natural to associate observables with the generators of such canonical transformations, similarly to the case of standard classical and quantum mechanics (see previous section). In particular, the ensemble Hamiltonian may be interpreted as the generator of time translations. However, it will be recalled from Chap. 1 that ensemble Hamiltonians must satisfy certain fundamental constraints, to ensure the conservation and positivity of probability. Similarly, one cannot associate an arbitrary function $A(P, S)$ with an observable: the infinitesimal canonical transformation generated by A,

$$P \to P + \varepsilon \frac{\delta A}{\delta S}, \quad S \to S - \varepsilon \frac{\delta A}{\delta P}, \tag{2.9}$$

must preserve the normalization and positivity of P. Hence, just as per Eqs. (1.18) and (1.25) for ensemble Hamiltonians, the conditions

$$A[P, S + c] = A[P, S], \quad \frac{\delta A}{\delta S} = 0 \text{ if } P(x) = 0 \tag{2.10}$$

must be satisfied for observables on continuous configuration spaces (and corresponding conditions for observables on discrete configuration spaces). The first of these conditions implies that only relative values of S have physical significance.

There is a further fundamental requirement which we will impose on observables, corresponding to the homogeneity property for ensemble Hamiltonians discussed in Sect. 1.4: that they be functionals which are homogeneous of degree one in P, i.e.,

$$A[\lambda P, S] = \lambda A[P, S], \tag{2.11}$$

where λ is an arbitrary positive constant. In particular, this property implies that A can consistently be interpreted as an ensemble average (see Sect. 1.4.3), i.e., the numerical value of A corresponds to the expectation value of the observable over the ensemble.

We are led therefore to the following definition of observables:

Definition The observables of a configuration ensemble are a set of functions (or functionals) of P and S satisfying the probability conservation, positivity and homogeneity properties in Eqs. (2.10) and (2.11).

Note that each of the conditions in Eqs. (2.10) and (2.11) is preserved by the Poisson bracket. First, defining $I[P, S] := \int dx\, P$, the conservation of probability is simply the requirement that I is invariant under allowed canonical transformations, i.e., that $\delta I = \varepsilon\{I, A\} = 0$. Hence, if it holds for two observables A and B, then it automatically holds for $\{A, B\}$ via the Jacobi identity, since

$$\{I, \{A, B\}\} = -\{A, \{B, I\}\} - \{B, \{I, A\}\} = 0. \tag{2.12}$$

Similarly, the positivity condition may be rewritten as $\delta P = \varepsilon\{P, A\} = 0$ whenever $P(x) = 0$ (otherwise $P(x)$ can be decreased below 0 by choosing the sign of ε appropriately), which again holds for $\{A, B\}$, if it holds for A and B, as a consequence of the Jacobi identity. Finally, it is straightforward to check that the Poisson bracket of two functionals which are homogeneous of degree one in P is also homogeneous of degree one in P. Hence, *it may assumed without loss of generality that the set of observables form a closed Lie algebra under the Poisson bracket.*

2.3 Examples

In the previous section we have given a precise definition of observables. We now consider a number of examples, including classical and quantum observables.

2.3.1 Position and Momentum Observables

Two examples of particular interest for continuous configuration spaces are position and momentum observables. Given the interpretation of observables as expectation values, following from the homogeneity property (2.11), an obvious definition for the ensemble position observable is

$$X[P, S] := \int dx\, Px. \tag{2.13}$$

Note that this observable generates the transformation

$$P \to P + \varepsilon \frac{\delta X}{\delta S} = P \tag{2.14}$$

via Eq. (2.9), and hence P trivially remains positive and normalised, as required by Eq. (2.10). The homogeneity property (2.11) is also trivially satisfied.

The definition of the ensemble momentum may be motivated by noting that in classical and quantum mechanics the momentum observable generates translations (for example, $\psi(x - \varepsilon) = e^{-i\varepsilon\cdot\hat{p}/\hbar}\psi(x)$ for a quantum wave function $\psi(x)$). Hence, identifying the ensemble momentum as the observable Π which generates translations, one has via Eq. (2.9) that

$$\varepsilon \cdot \frac{\delta \Pi}{\delta S} = \delta P = P(x - \varepsilon) - P(x) = -\varepsilon \cdot \nabla P(x), \tag{2.15}$$

and

$$\varepsilon \cdot \frac{\delta \Pi}{\delta P} = -\delta S = -[S(x - \varepsilon) - S(x)] = \varepsilon \cdot \nabla S(x). \tag{2.16}$$

for arbitrary infinitesimal translations ε on configuration space. The solution of these equations is, up to an arbitrary additive constant,

$$\Pi[P, S] := \int \mathrm{d}x\, P \nabla S, \tag{2.17}$$

for the ensemble momentum. In particular, this expression immediately yields $\delta\Pi/\delta P = \nabla S$, while under an infinitesimal variation $S \to S + \delta S$ one has

$$\delta \Pi = \Pi[P, S + \delta S] - \Pi[P, S] = \int \mathrm{d}x\, P\, \nabla(\delta S) = -\int \mathrm{d}x\, (\nabla P)\, \delta S, \tag{2.18}$$

which implies, via Eq. (A.1) of the Appendix, that one also has $\delta\Pi/\delta S = -\nabla P$ as required. Note that normalisation and positivity of P is trivially preserved under translations, implying that Eq. (2.10) is satisfied by $\Pi[P, S]$. Further, the homogeneity requirement (2.11) is satisfied by direct inspection.

It follows from Eq. (2.17) that $P\nabla S$ is a local momentum density for continuous configuration spaces, independently of whether the ensemble is classical, quantum, or something more general. This result (together with the identification of $-P\partial_t S$ as a local energy density in Sect. 1.4), helps to establish the physical role played by S in the formalism of ensembles on configuration space. However, to maintain full generality, S should not be regarded as a "momentum potential". This would go beyond what is required of a statistical theory. In particular, for an ensemble of classical particles with uncertainty described by the probability P, it will not be assumed that the momentum of a member of the ensemble is a well-defined quantity proportional to the gradient of S, as it is done in the usual deterministic interpretation of the Hamilton–Jacobi equation. This avoids forcing a similar deterministic interpretation in the quantum case. A deterministic picture can be recovered for classical ensembles precisely in those cases in which trajectories are operationally defined [3].

Finally, the Poisson bracket for the components of the ensemble position and momentum may be calculated from Eqs. (2.5), (2.13) and (2.17) as

$$\{X_m, \Pi_n\} = \delta_{mn} \tag{2.19}$$

which is the same result as for the Poisson bracket of two classical position and momentum observables [2]. A more general correspondence will be seen in the next example. This result is relevant to representations of the Galilean group of observables, as will be discussed in Sect. 2.5.

2.3.2 Classical Observables

In classical mechanics, observables corresponds to functions $f(x, p)$ on the classical phase space. We define the corresponding classical ensemble observable C_f by

$$C_f := \int \mathrm{d}x\, P f(x, \nabla S) \tag{2.20}$$

This is similar in form to a classical average, and clearly satisfies the homogeneity property (2.11). Hence, the numerical value of C_f may consistently be identified with the ensemble average of the corresponding function $f(x, p)$. Further, it is easily checked that C_f satisfies the required normalisation condition in Eq. (2.10)—the only dependence on S is via its gradient. The positivity condition in Eq. (2.10) is also satisfied, noting that

$$\begin{aligned}\frac{\delta C_f}{\delta S} &= \frac{\delta}{\delta S}\int dx\, P f(x, \nabla S) = P\,\frac{\partial f(x, \nabla S)}{\partial S} - \nabla\cdot\left[P\frac{\partial f(x, \nabla S)}{\partial \nabla S}\right]\\ &= -P\,\nabla\cdot\left[\frac{\partial f(x, \nabla S)}{\partial \nabla S}\right] - \nabla P\cdot\frac{\partial f(x, \nabla S)}{\partial \nabla S}\end{aligned} \tag{2.21}$$

(see the Appendix to this book regarding the calculation of variational derivatives). In particular, since P is non-negative, it must reach a global minimum at any point x for which $P(x) = 0$. Hence $\nabla P(x)$ also vanishes, and thus the last line vanishes at $P(x) = 0$ as required.

The Poisson bracket of any two classical observables C_f and C_g follows, using Eq. (2.5) and integration by parts with respect to x, as

$$\begin{aligned}\{C_f, C_g\} &= \int \mathrm{d}x\,\left[-f\nabla_x\cdot(P\nabla_p g) + g\nabla_x\cdot(P\nabla_p f)\right]\\ &= \int \mathrm{d}x\, P\left(\nabla_x f\cdot\nabla_p g - \nabla_x g\cdot\nabla_p f\right)\\ &= C_{\{f,g\}},\end{aligned} \tag{2.22}$$

where all quantities in the integrands are evaluated at $p = \nabla_x S$, and $\{f, g\}$ denotes the usual Poisson bracket for phase space functions. Hence, we have the remarkable result that

The Poisson bracket for classical ensembles on configuration space is isomorphic to the usual Poisson bracket on phase space.

This isomorphism between deterministic observables on phase space and ensemble observables on configuration space makes it possible to formulate thermodynamics on configuration space instead of phase space (see Chap. 4), and is crucial to the construction of hybrid quantum-classical systems (see Chaps. 8 and 9).

2.3.3 Quantum Observables

In quantum mechanics, the fundamental observables are represented by Hermitian operators. For Hermitian operator $\hat{M}$ acting on the Hilbert space spanned by the kets $\{|q\rangle\}$, the configuration space is defined by a choice of computational basis $\{|q\rangle\}$ (see Chap. 1), and we define the corresponding quantum ensemble observable $Q_{\hat{M}}$ by

$$\begin{aligned} Q_{\hat{M}} &:= \langle\psi|\hat{M}|\psi\rangle \\ &= \int \mathrm{d}q\,\mathrm{d}q'\,(PP')^{1/2}\mathrm{e}^{\mathrm{i}(S-S')/\hbar}\langle q'|\hat{M}|q\rangle, \end{aligned} \tag{2.23}$$

where $\psi(q) := \sqrt{P(q)}\,\mathrm{e}^{\mathrm{i}S(q)/\hbar}$, $P = P(q)$, $P' = P(q')$, etc. (and where integration with respect to q and q' is replaced by summation over any discrete portions of the quantum configuration space). This is just the quantum expectation value of $\hat{M}$ with respect to the wave function $\psi(q)$, and clearly satisfies the homogeneity property (2.11). Hence, the numerical value of $Q_{\hat{M}}$ may be identified with the ensemble average of the corresponding operator $\hat{M}$.

It follows immediately from Eq. (2.23) that $Q_{\hat{M}}$ also satisfies the normalisation condition in Eq. (2.10) since it only depends on differences of S at different points q and q' of configuration space. Further, the positivity condition is trivially satisfied for a discrete configuration space, while for the continuous case one has, under an infinitesimal variation $S \to S + \delta S$,

$$\begin{aligned} \delta Q_{\hat{M}} &= \int \mathrm{d}q\,\mathrm{d}q'\,(PP')^{1/2}\frac{\mathrm{i}}{\hbar}\left(\delta S - \delta S'\right)\mathrm{e}^{\mathrm{i}(S-S')/\hbar}\langle q'|\hat{M}|q\rangle \\ &= \int \mathrm{d}q\,\mathrm{d}q'\,(PP')^{1/2}\frac{\mathrm{i}}{\hbar}\left[\mathrm{e}^{\mathrm{i}(S-S')/\hbar}\langle q'|\hat{M}|q\rangle - \mathrm{e}^{\mathrm{i}(S'-S)/\hbar}\langle q|\hat{M}|q'\rangle\right]\delta S, \end{aligned}$$

immediately implying that

$$\frac{\delta Q_{\hat{M}}}{\delta S} = -\frac{1}{\hbar}\int \mathrm{d}q'\,(PP')^{1/2}\,\mathrm{Im}\left\{\mathrm{e}^{\mathrm{i}(S-S')/\hbar}\langle q'|\hat{M}|q\rangle\right\}, \tag{2.24}$$

which vanishes for $P(q) = 0$ as required.

To evaluate the Poisson bracket of any two quantum observables $Q_{\hat{M}}$ and $Q_{\hat{N}}$, it is convenient to first express the Poisson bracket in terms of the wave function $\psi(q)$ and its complex conjugate $\bar{\psi}(q)$. One has in particular for any real functional $A[P, S]$ that

$$\frac{\delta A}{\delta P} = \frac{\partial \psi}{\partial P}\frac{\delta A}{\delta \psi} + \frac{\partial \bar{\psi}}{\partial P}\frac{\delta A}{\delta \bar{\psi}} = \frac{1}{\bar{\psi}\psi}\,\mathrm{Re}\left\{\psi\frac{\delta A}{\delta \psi}\right\}, \tag{2.25}$$

$$\frac{\delta A}{\delta S} = \frac{\partial \psi}{\partial S}\frac{\delta A}{\delta \psi} + \frac{\partial \bar{\psi}}{\partial S}\frac{\delta A}{\delta \bar{\psi}} = -\frac{2}{\hbar}\,\mathrm{Im}\left\{\psi\frac{\delta A}{\delta \psi}\right\}, \tag{2.26}$$

and hence, noting $-ad + bc = \mathrm{Im}\{(a + \mathrm{i}b)(c - \mathrm{i}d)\}$, that

$$\{A, B\} = \frac{2}{\hbar}\,\mathrm{Im}\left\{\int \mathrm{d}q\,\frac{\delta A}{\delta \psi}\,\frac{\delta B}{\delta \bar{\psi}}\right\}. \tag{2.27}$$

A similar result holds for a discrete configuration space, with integration replaced by summation and variational derivatives by partial derivatives. Recalling that $\hat{M}$ and $\hat{N}$ are Hermitian, so that $\bar{\psi}\hat{M}\psi$ may be replaced by $\overline{(\hat{M}\psi)}\,\psi$ in Eq. (2.23), it immediately follows that

$$\{Q_{\hat{M}}, Q_{\hat{N}}\} = \frac{2}{\hbar}\,\mathrm{Im}\left\{\int \mathrm{d}q\,\overline{(\hat{M}\psi)}\hat{N}\psi\right\} = Q_{[\hat{M},\hat{N}]/(\mathrm{i}\hbar)}, \tag{2.28}$$

where $[\hat{M}, \hat{N}]$ denotes the usual quantum commutator $\hat{M}\hat{N} - \hat{N}\hat{M}$. Hence, in analogy to classical observables:

> The Poisson bracket for quantum ensembles on configuration space is isomorphic to the usual commutator on Hilbert space.

Thus, the Poisson bracket for ensemble observables unifies the standard classical and quantum brackets. This result is crucial to the construction of hybrid classical-quantum systems (see Chaps. 8 and 9).

2.4 Eigenensembles, Weak Values and Transition Probabilities

The examples discussed in the previous section show that the notion of ensemble observables encompasses both classical and quantum observables. It also allows for the generalisation of certain concepts which are important in quantum mechanics. In particular, as we show in this section, one may introduce generalisations of quantum mechanical eigenstates, eigenvalues, weak values and transition probabilities.

2.4.1 Eigensembles and Eigenvalues

We now want to introduce the notion of a state that is 'sharp' with respect to a particular observable, which we will call an eigenensemble. We will show that it is possible to give a general definition which fits into the canonical formalism of the theory of ensembles on configuration space. Such states are simply generalizations of stationary ensembles, which we will discuss first.

2.4.1.1 Stationary Ensembles

For ensemble Hamiltonians with no explicit time dependence, 'stationary ensembles' may be defined as those ensembles for which the dynamical properties of the ensemble are also time-independent. Recalling that only relative values of S are dynamically relevant (see Sect. 2.2), such ensembles must satisfy the conditions

$$P(x,t) = P(x,t'), \qquad S(x,t) - S(x',t) = S(x,t') - S(x',t'), \tag{2.29}$$

for all configurations x, x' and times t, t', which are equivalent to $\partial P/\partial t = 0$ and $S(x,t) = s(x) + f(t)$ for some functions s and f (the latter follows by noting the second condition implies $\partial[S(x,t) - S(x',t)]/\partial t = 0$, yielding $S(x,t) - S(x',t) = k(x,x')$ for some function k). Noting that $f''(t) = \partial^2 S/\partial t^2 = -(\partial/\partial t)(\delta\mathscr{H}/\delta P)$ (where $\delta\mathscr{H}/\delta P$ is replaced by $\partial\mathscr{H}/\partial P_j$ for discrete configuration spaces), and that the last term must vanish if the ensemble is time-independent, it follows that stationary ensembles are characterised by the conditions

$$\frac{\partial P}{\partial t} = 0, \qquad \frac{\partial S}{\partial t} = -E, \tag{2.30}$$

for some constant E.

The above conditions clearly generalise the concept of a stationary state in quantum mechanics, where E is a corresponding energy eigenvalue. In particular, for this case Eq. (2.30) reduces to, using Eqs. (2.1), (2.6) and (2.23) with $\hat{M} = \hat{H}$, the stationary Schrödinger equation $i\hbar\partial_t|\psi\rangle = \hat{H}|\psi\rangle = E|\psi\rangle$. In classical mechanics, these conditions are equivalent to postulating a stationary state with time-independent P and a solution of the Hamilton–Jacobi theory of the special form $S(x,t) = -Et + W(x)$, where E is the energy of the state and $W(x)$ is sometimes called Hamilton's characteristic function [2]. We will meet stationary ensembles again in Chap. 4 (for thermal mixtures) and Chap. 8 (for hybrid quantum-classical ensembles).

2.4.1.2 General Eigensembles

Just as stationary ensembles generalise quantum stationary states, we may generalise the notion of quantum eigenstates as follows.

Definition For a given observable A, the configuration ensemble (P, S) is defined to be an 'eigenensemble' of A if and only if the physical properties of the ensemble are invariant under the canonical transformation generated by A.

To apply this definition, note first that the probability density P is in principle measurable, and hence must be invariant, i.e.,

$$\delta P(x) = \varepsilon\{P(x), A\} = 0. \tag{2.31}$$

Second, since physical properties are invariant under addition of a constant to S, only relative values of S are required to be invariant under transformations generated by A, i.e.,

$$\delta S(x) - \delta S(x') = \varepsilon\{S(x) - S(x'), A\} = 0 \tag{2.32}$$

for all x and x'. It follows that (P, S) is an eigenensemble of observable A if and only if

$$\frac{\delta A}{\delta S} = 0, \qquad \frac{\delta A}{\delta P} = \text{constant} = \alpha. \tag{2.33}$$

The constant α will be called the *eigenvalue* of A for such an eigenensemble.

A solution of Eq. (2.33) for a particular eigenvalue α will be denoted by (P_α, S_α). It will be seen in Sect. 2.4.2 below that the value of A on an eigenensemble is equal to the corresponding eigenvalue, i.e.,

$$A(P_\alpha, S_\alpha) = \alpha. \tag{2.34}$$

Note that Eq. (2.33) reduces to the definition of a stationary state in Eq. (2.30) when one identifies A with the ensemble Hamiltonian $\mathscr{H}$, and α with the energy E. For the quantum observable $Q_{\hat{M}}$ in Eq. (2.23) it reduces to the definition of an eigenstate of $\hat{M}$. Of course, for more general functions A of P and S there may be no corresponding eigensembles.

2.4.2 *Weak Values and Local Densities*

Differentiating the homogeneity property $A[\lambda P, S] = \lambda A(P, S)$ in Eq. (2.11) with respect to λ, and setting $\lambda = 1$, yields the numerical equivalence

$$A[P, S] = \int \mathrm{d}x\, P \frac{\delta A}{\delta P}. \tag{2.35}$$

Thus, each observable A has an associated *local density* $P(\delta A/\delta P)$ on the configuration space. For the case of the ensemble Hamiltonian this is a local energy density, $-P\partial_t S$, as noted previously in Chap. 1.

The existence of such local densities may be used to show that A may be consistently interpreted as an ensemble expectation value (the argument is identical to that in Sect. 1.4.3 for ensemble Hamiltonians, and does *not* require any interpretation for the local density itself). Further, Eqs. (2.33) and (2.35) immediately yield Eq. (2.34) for eigensembles of A.

Equation (2.35) leads to a further remarkable result: a far-reaching generalisation of the notion of the 'weak value' of an observable in quantum mechanics [4, 5]. In particular, we will define the weak value of an observable A, for an *arbitrary* configuration ensemble (P, S), by the function

$$A^{\mathrm{w}}(x) := \frac{\delta A}{\delta P} \tag{2.36}$$

on the configuration space (with the variational derivative replaced by a partial derivative for discrete configuration spaces).

Note first that the average of the weak value over the ensemble follows immediately from Eq. (2.35) as

$$\langle A^{\mathrm{w}} \rangle := \int dx\, P(x)\, A^{\mathrm{w}}(x) = A[P, S]. \tag{2.37}$$

Thus, the expectation values of A and A^{w} are equal. For eigensembles of A the stronger result $A^{\mathrm{w}} = \alpha$ holds via Eq. (2.34).

Second, for the classical ensemble observable C_f defined in Eq. (2.20), the corresponding weak value follows as

$$C_f^{\mathrm{w}}(x) = f(x, \nabla S). \tag{2.38}$$

Thus, the classical weak value is equal to the classical phase space function $f(x, p)$ evaluated at $p = \nabla S$.

Third, for the quantum ensemble observable $Q_{\hat{M}}$ defined in Eq. (2.23), the corresponding weak value follows via Eqs. (2.25) and (2.36) as

$$\begin{aligned} Q_{\hat{M}}^{\mathrm{w}}(q) &= \frac{1}{\bar{\psi}(q)\psi(q)} \operatorname{Re}\left\{ \psi(q) \frac{\delta Q_{\hat{M}}}{\delta \psi} \right\} \\ &= \operatorname{Re}\left\{ \frac{\langle q|\hat{M}|\psi\rangle}{\langle q|\psi\rangle} \right\}, \end{aligned} \tag{2.39}$$

where the property $\delta Q_{\hat{M}}/\delta\psi = \overline{\hat{M}\psi(q)}$ has been used, following from the expression

$$Q_{\hat{M}} = \int dq\, \bar{\psi}(q)\hat{M}\psi(q) = \int dq\, \overline{\hat{M}\psi(q)}\psi(q) \tag{2.40}$$

for Hermitian operators. Equation (2.39) may be recognised as the quantum weak value of $\hat{M}$ [4, 5]—thus justifying the use of the terminology 'weak value' for the general case in Eq. (2.36).

As originally introduced by Aharonov and Vaidman, weak values correspond to the average outcome of an apparatus weakly coupled to $\hat{M}$ and postselected by measurement result $\hat{Q} = q$ in the computational basis $\{|q\rangle\}$[1] [4, 5]. An alternative characterisation of $Q^{\mathrm{w}}_{\hat{M}}$ is that it provides the best possible estimate of the value of $\hat{M}$ from a measurement in the computational basis on state $|\psi\rangle$ [6–8]. An excellent review on the interpretation of quantum weak values has been given recently by Dressel [9].

It would be of great interest to assess the degree to which the above interpretations can be applied in the general context of arbitrary observables for ensembles on configuration space. We do not address this issue in detail here, but note that it is natural, in this context, to consider the *weak observable* $A^{\mathrm{w}}[P, S]$, defined by

$$A^{\mathrm{w}}[P] := \int \mathrm{d}x\, P(x)\, A^{\mathrm{w}}(x) \tag{2.41}$$

(with integration replaced by summation for discrete configuration spaces), treating $A^{w}(x)$ as a fixed function on configuration space. The weak observable only depends on the configuration parameter x, and from Eq. (2.37) is numerically equal to $A[P, S]$. The weak observable corresponds to the average weak measurement outcomes in the first interpretation above, while the difference between the weak observable and A is relevant to defining the optimal estimate in the second interpretation above. The connection of weak values to weak measurements is explored further in Sect. 3.5 of Chap. 3.

2.4.3 Transition Probabilities

We have seen that ensemble observables allow for general definitions of eigensembles, eigenvalues and weak values, which generalize the corresponding concepts in quantum theory. We now want to look briefly at how generalised transition probabilities might be defined.

Suppose first that a particular configuration ensemble, (P, S), is an eigensemble with respect to some observable G, with corresponding eigenvalue γ. The notation

[1]Weak values are defined by some authors as $\frac{\langle q|\hat{M}|\psi\rangle}{\langle q|\psi\rangle}$; however, it is the real part of this quantity that has a direct interpretation in terms of weak measurements.

(P_γ, S_γ) would be better suited here, but we will simply use (P, S) when it can not lead to confusion, to simplify the notation. We thus have (see Sect. 2.4.1)

$$\frac{\delta G}{\delta S} = 0, \quad \frac{\delta G}{\delta P} = \gamma, \quad G[P, S] = \langle \delta G/\delta P \rangle = \gamma. \tag{2.42}$$

Consider further a second observable F, which has various possible measurement values parameterized by a variable ϕ. It will *not* be assumed at this stage that the values of ϕ are also eigenvalues of F. We can now ask the following question: *What is the probability of obtaining measurement result $F = \phi$ for the eigensemble of G having eigenvalue γ*? This probability will be denoted by $w(\phi|\gamma)$.

To answer this question, consider first some function $f(\phi)$ of the possible measurement outcomes. Then, the corresponding expectation value of this function follows as

$$\langle f(\phi) \rangle = \int \mathrm{d}\phi \, w(\phi|\gamma) f(\phi). \tag{2.43}$$

It is natural to now make the assumption that this expectation value *is itself* the expectation value of some observable. This amounts to a 'completeness' assumption for the set of observables. We will call this observable $A_{f(F)}[P, S]$. Thus, the equality $A_{f(F)} = \langle f(\phi) \rangle$ is satisfied.

It follows immediately from Eq. (2.43) that one has the general relation

$$\int \mathrm{d}\phi \, w(\phi|\gamma) f(\phi) = \langle f(\phi) \rangle = A_{f(F)} = \int \mathrm{d}x P \, \frac{\delta A_{f(F)}}{\delta P}. \tag{2.44}$$

for an *arbitrary* function f. The task then is to choose a particular set of functions f which allows this relationship to be inverted, so as to solve for the value of the transition probability $w(\phi|\gamma)$. For example, one could choose a set of orthogonal polynomials (e.g., Legendre polynomials) in the case of bounded sets of measurement outcomes. Here we consider another choice, the relatively simple 'Fourier' choice $f_z(\phi) = \mathrm{e}^{\mathrm{i}z\phi}$. Hence the left hand side of the above relationship is a Fourier transform. We can then apply the inverse transform with respect to z, to obtain the explicit solution

$$w(\phi|\gamma) = \frac{1}{2\pi} \int \mathrm{d}z \, \mathrm{d}x \, P(x) \, \mathrm{e}^{-\mathrm{i}z\phi} \, \frac{\delta A_{f_z(F)}}{\delta P}. \tag{2.45}$$

For discrete-valued observables, a discrete Fourier transform would be appropriate.

However, the solution given by Eq. (2.45) remains formal until we specify how the functional $A_{f(F)}$ is to be constructed from a given observable F and function f. We discuss two approaches for doing this.

The first approach is to give $A_{f(F)}$ an *operational* definition. For example, for both quantum and classical observables weak values can be *measured* following the approach proposed by Aharonov and Vaidman, via a coupling to a weak meter followed by a position measurement [5] (see also Sects. 2.4.2 and 3.5). Now, suppose it is possible to measure weak values more generally, by a similar well-defined procedure—e.g., $A^{\mathrm{w}}_{f(F)}(x)$ might be measurable via coupling to a weak F-meter followed by a position measurement. Equation (2.43) can then be rewritten in the operationally well-defined form

$$w(\phi|\gamma) = \frac{1}{2\pi}\int \mathrm{d}z\,\mathrm{d}x P(x)\,\mathrm{e}^{-\mathrm{i}z\phi}\,A^{\mathrm{w}}_{f(F)}(x). \tag{2.46}$$

A different, more formal approach to inverting Eq. (2.43) requires defining the observable F^k for $k = 2, 3, \ldots$, as this would allow one to construct most observables $A_{f_z(F)}$ of interest. This effectively corresponds to defining a product algebra on the set of observables. We carry out this construction for the classical and quantum observables defined in Sect. 2.3. For the classical observable C_g, where g is some phase space function $g(x, p)$, we define

$$f(C_g) := C_{f(g)}. \tag{2.47}$$

Thus, for example, one has

$$(C_g)^2[P, S] = \int \mathrm{d}x\,P\,g(x, \nabla S)^2. \tag{2.48}$$

For the quantum observable $Q_{\hat{M}}$, where $\hat{M}$ is some Hermitian operator, we define

$$f(Q_{\hat{M}}) := Q_{f(\hat{M})}. \tag{2.49}$$

Thus, for example, the observable corresponding to square of the momentum is

$$(Q_{\hat{p}})^2[P, S] = \int \mathrm{d}x\,P\left[|\nabla S|^2 + (\hbar^2/4)|\nabla \log P|^2\right]. \tag{2.50}$$

Thus transition probabilities may be calculated via powers of observables in these cases.

2.5 Symmetries and Transformations

The Poisson bracket satisfies all the properties required of a Lie algebra, i.e., linearity, asymmetry and the Jacobi identity:

$$\{A + B, C\} = \{A, C\} + \{B, C\}, \qquad \{A, B\} = -\{B, A\}, \tag{2.51}$$

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0, \tag{2.52}$$

as may easily be verified directly from Eqs. (2.2) and (2.5). Hence the set of canonical transformations, generated by a set of observables closed under the Poisson bracket, form a Lie group (for quantum observables this group is of course the usual unitary transformations). This allows us to describe systems with symmetries. We will consider two examples below: nonrelativistic particles and rotational bits.

2.5.1 Nonrelativistic Particles

Consider first the possible descriptions of a free nonrelativistic particle—whether classical, quantum or otherwise. We will take the configuration space to be the Euclidean space R^3. To describe such a particle, we look for a realization of the Galilean group in terms of the algebra of Poisson brackets. The Galilean group has 10 generators: A_i which generate spatial displacements, H which generates time displacements, L_i which generate spatial rotations, and G_i which generate Galilean transformations ("boosts"), with $i = 1, 2, 3$. These generators have to satisfy the Poisson bracket relations [10]

$$\{H, A_i\} = 0, \qquad \{H, L_i\} = 0, \tag{2.53}$$

$$\{L_i, A_j\} = \varepsilon_{ijk} A_k, \qquad \{L_i, L_j\} = \varepsilon_{ijk} L_k, \qquad \{L_i, G_j\} = \varepsilon_{ijk} G_k, \tag{2.54}$$

$$\{A_i, A_j\} = 0, \qquad \{G_i, G_j\} = 0, \qquad \{G_i, A_j\} = m\delta_{ij}, \qquad \{G_i, H\} = A_i, \tag{2.55}$$

where m is the mass of the particle, and $\varepsilon_{ijk} = 1\ (= -1)$ for even (odd) permutations i, j, k of 1, 2, 3 and vanishes otherwise. Note the first line implies that H transforms as a scalar under translations and rotations, while the second line implies that A_i, L_i, and G_i transform as vectors.

In the framework of ensembles on configuration space, these generators are represented by suitable observables. For spatial displacements and rotations one finds that

$$A_i = \Pi_i[P, S] = \int d^3x\, P\ (\partial_i S)\,, \qquad L_i = \int d^3x\, P\ \left(\varepsilon_{ijk}\, x_j\, \partial_k S\right), \tag{2.56}$$

up to additive constants. These are the ensemble momentum and angular momentum observables. The former observable, $\Pi[P, S]$, was derived in Sect. 2.3.1, and the latter may be similarly obtained by considering infinitesimal rotations of P and S. Further, for the Galilean boost transformations it is natural to choose the observables

$$G_i = \int d^3x\, P\ (m x_i - t\partial_i S) = m X_i[P, S] - t\Pi_i[P, S], \tag{2.57}$$

where t is the time. This follows from the standard definition $G_i = (mX_i - tA_i)$ in classical mechanics [10], together with the natural choice $X_i = \int d^3x\, P\, x_i$ for the position observable of an ensemble on configuration space as per Eq. (2.13).

The above results do not fully determine the form of H, which will of course, since it generates infinitesimal displacements in time, be identified with the ensemble Hamiltonian $\mathscr{H}$. It is straightforward to check from the above equations that the general solution is of the form

$$H = \mathscr{H}[P, S] := \int dx\, P\, \frac{|\nabla S|^2}{2m} + K[P, S], \tag{2.58}$$

where K is any observable invariant under translations, rotations and boosts, i.e., K is a Galilean scalar. Solutions include both the classical ensemble Hamiltonian for a free particle (see Sect. 1.2),

$$H = \mathscr{H}_C[P, S] = \int d^3x\, P\, \frac{|\nabla S|^2}{2m} \tag{2.59}$$

corresponding to $K \equiv 0$, and the quantum ensemble Hamiltonian for a free particle (see Sect. 1.2),

$$H = \mathscr{H}_Q[P, S] = \int d^3x\, P \left[\frac{|\nabla S|^2}{2m} + \frac{\hbar^2 |\nabla \log P|^2}{8m} \right] \tag{2.60}$$

corresponding to $K = (\hbar^2/8m) F[P]$, where $F[P]$ is the Fisher information of P [11] (see also Chap. 5). A more general solution corresponds to the choice

$$K[P, S] = \int dx\, P\, k(|\nabla \log P|, \nabla^2 \log P, \dots), \tag{2.61}$$

where k is an arbitrary function of scalars formed by the derivatives of $\log P$. Note that all the above generators satisfy the homogeneity condition, Eq. (2.11), and hence have clear interpretations as expectation values.

2.5.2 *Rotational Bits*

A quantum mechanical spin-half system may be characterised as having a set of two-valued observables which generate infinitesimal rotations in three dimensions. We want to consider such a two-level system, but now within the formalism of ensembles on configuration space. The generator of rotation about a given direction will be identified with the measurement of spin in that direction. Such a system may be called a *rotational bit* or *robit*, to distinguish it from the standard quantum qubit.

The observable corresponding to a measurement in unit direction $\mathbf{n}$ thus has the form $L \cdot \mathbf{n}$, where $L = (L_1, L_2, L_3)$ satisfies the $so(3)$ Lie algebra,

$$\{L_j, L_k\} = \varepsilon_{jkl} L_l, \tag{2.62}$$

for $j, k = 1, 2, 3$.

It convenient to define the probability distribution P in terms of the possible measurement outcomes of spin in the z-direction, which may be labelled by $\pm 1/2$. Thus, $P \equiv \{P_+, P_-\}$, where P_α denotes the probability of measuring spin value $\alpha/2$ in the z-direction. The canonically conjugate quantities are therefore labelled as $S \equiv \{S_+, S_-\}$.

Note that the identification of generators with expectation values immediately fixes the form of L_3. In particular, the average value of spin measurements in the z-direction may be calculated directly from the probability distribution,

$$L_3(P, S) = s(P_+ - P_-) = (P_+ - P_-)/2. \tag{2.63}$$

where $s = 1/2$ for spin-half particles (note for the quantum case we are effectively choosing units in which $\hbar = 1$).

We explore robits in detail in Chap. 7, where we develop theories for a single robit and pairs of robits. Here however we restrict to a single robit and focus on the problem of representing rotations on a *discrete* configuration space.

2.5.2.1 Reduced Phase Space for a Two-Level System

The fundamental variables for a two-level system are $\{P_+, P_-, S_+, S_-\}$, thus the phase space is four-dimensional. However, since $\sum_k P_k = 1$ is a quantity that is conserved, it is possible to describe the system in a reduced phase space. To do this, introduce coordinates

$$\begin{aligned} q_0 &= (P_+ + P_-)/2, \\ q_1 &= (P_+ - P_-)/2, \\ p_0 &= S_+ + S_-, \\ p_1 &= S_+ - S_-. \end{aligned} \tag{2.64}$$

It is easy to check that this transformation is a canonical transformation. Since the P_k are probabilities we must set $q_0 = 1/2$. In these coordinates, the conditions of probability conservation and homogeneity in Eqs. (2.10) and (2.11) require that observables G be of the form

$$G(q_1, q_2, p_1, p_2) = 2q_0 F(q_0^{-1} q_1/2, p_1), \tag{2.65}$$

where F is an arbitrary function and factors of 2 have been included for convenience. Since p_0 does not appear in G, the equations of motion lead to q_0 being a constant of the motion, as required.

It is now straightforward to describe the system in a phase space of dimension $4 - 2 = 2$. In particular, setting $q_0 = 1/2$ in the expression for G leads to

$$G(q_1, p_1) = F(q_1, p_1). \tag{2.66}$$

Thus we have identified the true degrees of freedom of the system, q_1 and p_1.

2.5.2.2 Two-Level System with $SO(3)$ Symmetry

We now look for the most general representation of $so(3)$ on this two-dimensional phase space. The generators must satisfy the Poisson brackets of Eq. (2.62), with the condition of Eq. (2.63), where the latter corresponds to

$$L_3 = q_1. \tag{2.67}$$

Equations (2.62) and (2.67) lead to

$$L_1 = -\frac{\partial L_2}{\partial p_1}, \tag{2.68}$$

$$L_2 = \frac{\partial L_1}{\partial p_1}, \tag{2.69}$$

$$L_3 = q_1 = \frac{\partial L_1}{\partial q_1}\frac{\partial L_2}{\partial p_1} - \frac{\partial L_1}{\partial p_1}\frac{\partial L_2}{\partial q_1}. \tag{2.70}$$

It is convenient to define $Z := L_1 - \mathrm{i}\, L_2$, and write Eqs. (2.68) and (2.69) as the single complex equation

$$\frac{\partial Z}{\partial p_1} = \mathrm{i}\, z. \tag{2.71}$$

Equation (2.71) has the general solution $Z = \exp\{\mathrm{i}p_1 + a(q_1) + \mathrm{i}b(q_1)\}$, where a and b are real functions of q_1. Thus

$$L_1 = \mathrm{e}^{a(q_1)} \cos(p_1 + b(q_1)), \qquad L_2 = -\mathrm{e}^{a(q_1)} \sin(p_1 + b(q_1)). \tag{2.72}$$

Substitution into Eq. (2.70) then leads to

$$L_1 = \sqrt{c^2 - q_1^2}\,\cos(p_1 + b(q_1)), \tag{2.73}$$

$$L_2 = -\sqrt{c^2 - q_1^2}\,\sin(p_1 + b(q_1)), \tag{2.74}$$

$$L_3 = q_1 \tag{2.75}$$

where c is a constant and b an arbitrary function of q_1.

To fix the value of c^2, we impose the condition that the probability remain positive. We consider an arbitrary ensemble Hamiltonian $H(L)$ which is a function of the generators of the $so(3)$ Lie algebra and calculate the change induced on q_1 by the action of H. Evaluation of the Poisson bracket leads to

$$\frac{\partial q_1}{\partial t} = \sqrt{c^2 - q_1^2}\left[-\frac{\partial H}{\partial L_1}\sin(p_1 + b) - \frac{\partial H}{\partial L_2}\cos(p_1 + b)\right], \tag{2.76}$$

The condition that the probability remain positive requires

$$\begin{aligned} \frac{\partial P_+}{\partial t} &= +\frac{\partial q_1}{\partial t} = 0 \quad \text{when} \quad q_1 = -\frac{1}{2}, \\ \frac{\partial P_-}{\partial t} &= -\frac{\partial q_1}{\partial t} = 0 \quad \text{when} \quad q_1 = +\frac{1}{2}. \end{aligned} \tag{2.77}$$

The positivity conditions have to be valid for all possible choices of H, which leads immediately to $c^2 = 1/4 = q_0^2$.

Thus, the general solution for the L_k is given by Eqs. (2.73)–(2.75) with $c^2 = 1/4$. One can see that the L_k still depend on the arbitrary function $b(q_1)$. However, we can always set $b(q_1) = 0$ via the simple canonical transformation

$$q_1 \to q_1, \qquad p_1 \to p_1 - b(q_1), \tag{2.78}$$

which obviously preserves the condition of Eq. (2.67). This allows us to write the generators of $so(3)$ in their simplest form,

$$L_1 = \sqrt{1/4 - q_1^2}\,\cos(p_1) = \sqrt{P_+ P_-}\,\cos(S_+ - S_-), \tag{2.79}$$

$$L_2 = -\sqrt{1/4 - q_1^2}\,\sin(p_1) = -\sqrt{P_+ P_-}\,\sin(S_+ - S_-), \tag{2.80}$$

$$L_3 = q_1 = (P_+ - P_-)/2. \tag{2.81}$$

We will show in Chap. 7 that a single robit is equivalent to a single quantum mechanical qubit. Notice however that we have derived the theory of a single robit without making any assumptions which are particular to quantum mechanics. We will develop this theme further in Chap. 7. In the case of a pair of robits, which we also discuss in Chap. 7, such an equivalence is no longer automatically fulfilled, but one may introduce further assumptions involving locality and a restriction of the functional form of the generators to obtain a similar equivalence to a pair of qubits.

2.6 Constraints and Superselection Rules

In the usual quantization of a classical system subject to constraints, each classical constraint is mapped to a linear operator constraint on the wavefunction, of the form $\hat{C}\psi = 0$ [12–14]. Thus, in standard quantum mechanics, one usually restricts to constraints that are *linear* in the wave function. However, in the more general context of ensembles on configuration space, it is natural to consider general constraints formulated in terms of P and S [15]—which, for quantum ensembles, will typically be *nonlinear* in the wave function. In particular, we define a constraint in a very general way, as any equation of the form

$$C(P, S) = 0 \tag{2.82}$$

that is required to hold at all times. This is completely analogous to the treatment of constraints in classical phase space physics [2, 13], and restricts the evolution to a submanifold of the fundamental variables (P, S). It will be seen that constraints of the above form have a fundamental role to play in quantum theory, even when they cannot be rewritten in the linear form $\hat{C}\psi = 0$. More generally, they may be interpreted as a generalisation of quantum superselection rules [15].

The Schrödinger equation for a quantum system is linear, implying that the superposition of any two solutions is also a solution. However, some combinations of states have never been observed, including coherent superpositions of integer and half-integer spins, electric charges, and Schrödinger's cat. Possible explanations for why such superpositions are not observed fall into two logical categories:

1. *measurement superselection rules*: such superpositions may be allowed, but physical limitations on measurement prevent their observation;
2. *state superselection rules*: such superpositions are not physically allowed.

State superselection rules are stronger than measurement superselection rules (one cannot observe what does not exist), and are clearly constraints on possible states of quantum ensembles. However, they are not *linear* constraints. For example, a superselection rule restricting possible wave functions of a quantum system to a set of orthogonal subspaces of Hilbert space (corresponding, e.g., to different spin values), with corresponding projection operators $\{\hat{E}_j\}$, is equivalent to the nonlinear constraint

$$\sum_j \langle\psi|\hat{E}_j|\psi\rangle^2 = 1 \tag{2.83}$$

on the wave function.

In this section, we present an example of a simple constraint on P and S that may be applied to both classical and quantum ensembles, and which in the latter case acts to rule out superpositions of energy eigenstates. Thus, this example shows how constraints of the form of Eq. (2.82) may be interpreted as generalised state superselection rules.

In particular, consider the rather simple canonical constraint

$$J := P\,\nabla S = 0. \tag{2.84}$$

This constraint is local, invariant under the transformation $S \to S + c$, and may be physically interpreted as the requirement that the ensemble momentum density vanishes everywhere. Note that for quantum ensembles it can be re-expressed as $\mathrm{Im}\,\bar{\psi}\nabla\psi = 0$, which clearly cannot be put in the linear form $\hat{C}\psi = 0$ of the standard approach to quantum constraints.

To investigate constraint (2.84) for a *classical* ensemble of particles, note that consistency with the equations of motion requires $\partial J/\partial t = 0$. The equations of motion for the ensemble (see Sect. 1.2) yield the secondary constraint

$$\begin{aligned} 0 = \partial(P\nabla S)/\partial t &= (\partial P/\partial t)\nabla S + P(\partial(\nabla S)/\partial t) \\ &= -[\nabla \cdot (P\nabla S)]\nabla S - P\,\nabla[|\nabla S|^2/(2m) + V] \\ &= -P\nabla V. \end{aligned} \tag{2.85}$$

Hence the classical force, $-\nabla V$, vanishes over the support of the ensemble, i.e., the ensemble is constrained to be stationary. Note in particular that if the potential energy has a single minimum, then the constraint requires the ensemble to be concentrated solely at this minimum, i.e., the ensemble must occupy the classical ground state.

In contrast, for a *quantum* ensemble of particles, Eq. (2.84) requires that ∇S vanishes on the support of the wavefunction, and hence that S has no spatial dependence for $P \neq 0$. Secondary constraints arising from consistency with the equations of motion can be determined similarly to the classical case above. However, it is simpler to directly substitute the ansatz $S(x,t) = -f(t)$ into the Schrödinger equation and use the continuity equation to obtain the secondary constraints

$$\dot{f}P^{1/2} = \left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]P^{1/2}, \qquad \partial P/\partial t = 0 \tag{2.86}$$

respectively. Differentiating the first of these with respect to time and applying the second implies that $\dot{f} = E =$ constant, and hence these constraints are equivalent to the time-independent Schrödinger equation

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi. \tag{2.87}$$

Thus the quantum ensemble is required to be in an energy eigenstate.

It is seen that in both the classical and quantum cases, the primary constraint in Eq. (2.29) leads to the requirement that the ensemble is stationary as per the definition in Eq. (2.30). In the quantum case this immediately yields a state superselection rule: *superpositions of states of different energy are forbidden*. Thus this constraint provides a very simple example of how canonical constraints can lead to superselection-type rules for quantum ensembles. Further examples and discussion of constraints are given in [15].

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