

That Strange Procedure Called Quantisation

Domenico Giulini
University of Freiburg
Department of Physics
Hermann-Herder-Strasse 3
D-79104 Freiburg,
Germany

Abstract

This is a pedagogical and (almost) self-contained introduction into the Theorem of Groenewold and van Howe, which states that a naive transcription of Dirac's quantisation rules cannot work. Some related issues in quantisation theory are also discussed. First-class constrained systems are briefly described in a slightly more 'global' fashion.¹

1 Introduction and Motivation

In my contribution I wish to concentrate on some fundamental issues concerning the notion of *quantisation*. Nothing of what I will say is new or surprising to the experts. My intention is rather a pedagogical one: to acquaint the non-experts with some of the basic structural results in quantisation theory, which I feel should be known to anybody who intends to 'quantise' something. A central result is the theorem of Groenewold and van Hove, which is primarily a no-go result, stating that the most straightforward axiomatisation of Dirac's informally presented 'canonical' quantisation rules runs into contradictions and therefore has to be relaxed. The constructive value of this theorem lies in the fact that its proof makes definite suggestions for such relaxations. This helps to sharpen one's expectations on the quantisation concept in general, which is particularly important for Quantum Gravity since here sources for direct physical input are rather scarce. Expectations on

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what Quantum Gravity will finally turn out to be are still diverse, though more precise pictures now definitely emerge within the individual approaches, as you will hopefully be convinced in the other lectures [14, 15, 17], so that reliable statements about similarities and differences on various points can now be made. The present contribution deliberately takes focus on a very particular and seemingly formal point, in order to exemplify in a controllable setting the care needed in formulating ‘rules’ for ‘quantisation’. At the end I will also briefly consider constrained systems from a slightly more ‘global’ point of view. Two appendices provide some technical aspects.

How do you recognize *quantum* theories and what structural elements distinguish them from so-called classical ones? If someone laid down, in mathematical terms, a theory of ‘something’ before you, what features would you check in order to answer this question? Or would you rather maintain that this question does not make good sense to begin with? Strangely enough, even though quantum theories are not only known to be the most successful but also believed to be the most fundamental theories of physics, there seems to be no unanimously accepted answer to any of these questions. So far a working hypothesis has been to *define* quantum theories as the results of some ‘quantisation procedures’ after their application to classical theories. One says that the classical theory (of ‘something’) ‘gets quantised’ and that the result is the quantum theory (of that ‘something’). This is certainly the way we traditionally understand Quantum Mechanics and also a substantial part of Quantum Field Theory (for more discussion on this point, that also covers interesting technical issues, I recommend [12]). As an exception—to a certain degree—I would list Local Quantum Field Theory [10], which axiomatically starts with a general kinematical framework for Poincaré invariant quantum field theories without any a priori reference to classical theories. Although this can now be generalised to curved spacetimes, it does not seem possible to eliminate the need of some such fixed (i.e. non-dynamical) background. Hence this approach does not seem to be able to apply to background independent dynamical fields, like gravity.

The generally accepted quantisation procedures I have in mind here can be roughly divided into three groups, with various interrelations:

- Hilbert-space based methods, like the standard canonical quantisation programme,
- algebraic methods based on the notion on observables, like \star -product quantisation or C^* -algebra methods,
- path integral methods.

Given the success of Quantum Mechanics (QM) it was historically, and still is, more than justified to take it as paradigm for all other quantum theories (modulo extra technical inputs one needs to handle infinitely many degrees of freedom). Let us therefore take a look at QM and see how quantisation may, or may not, be understood. In doing this, I will exclusively focus on the traditional ‘canonical’ approaches to quantisation.

2 Canonical Quantisation

Historically the rules for ‘canonical quantisation’ were first spelled out by Dirac in his famous book on QM [3]. His followers sometimes bluntly restated these rules by the symbolic line,

$$\{\cdot, \cdot\} \mapsto \frac{-i}{\hbar}[\cdot, \cdot], \quad (1)$$

which is to be read as follows: map each classical observable (function on phase space) f to an operator \hat{f} in a Hilbert space \mathcal{H} (typically $L^2(Q, d\mu)$, where Q is the classical configuration space and $d\mu$ the measure that derives from the Riemannian metric thereon defined by the kinetic energy), in such a way that the Poisson bracket of two observables is mapped to $-i/\hbar$ times the commutator of the corresponding operators, i.e., $\widehat{\{f_1, f_2\}} = \frac{-i}{\hbar}[\hat{f}_1, \hat{f}_2]$. This is also facetiously known as ‘quantisation by hatting’. But actually Dirac was more careful; he wrote [3] (my emphasis; P.B. denotes ‘Poisson Brackets’)

‘The strong analogy between quantum P.B. [i.e. commutators] and classical P.B. leads us to make the assumption that the quantum P.B., or at any rate the simpler ones of them, have the same values as the corresponding classical P.B.s.’

PAUL DIRAC, 1930

Clearly these words demand a specific interpretation before they can be called a (well defined) quantisation programme.

2.1 The classical stage

Associated to a classical Hamiltonian dynamical system of n degrees of freedom is a $2n$ -dimensional manifold, P , the space of states or ‘phase space’ (sometimes identified with the space of solutions to Hamilton’s equations, if the latter pose a well defined initial-value problem). Usually—but not always—it comes equipped with a preferred set of $2n$ functions, (q^i, p_i) , $i = 1 \cdots n$, called coordinates and

momenta respectively. In addition, there is a differential-geometric structure on P , called *Poisson Bracket*, which gives a suitable subspace $\mathcal{F} \subseteq C^\infty(P)$ of the space of real-valued, infinitely differentiable functions the structure of a Lie algebra. See Appendix 1 for more information on the geometric structures of classical phase space and Appendix 2 for the general definition of a Lie algebra. Exactly what subspace is ‘suitable’ depends of the situation at hand and will be left open for the time being. In any case, the Poisson Bracket is a map

$$\{\cdot, \cdot\} : \mathcal{F} \times \mathcal{F} \rightarrow \mathcal{F}, \quad (2)$$

which satisfies the following conditions for all $f, g, h \in \mathcal{F}(P)$ and $\lambda \in \mathbb{R}$ (which make it precisely a real Lie algebra):

$$\{f, g\} = -\{g, f\} \quad \text{antisymmetry,} \quad (3)$$

$$\{f, g + \lambda h\} = \{f, g\} + \lambda \{f, h\} \quad \text{linearity,} \quad (4)$$

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0 \quad \text{Jacobi identity.} \quad (5)$$

In the special coordinates (q^i, p_i) it takes the explicit form (cf. Appendix 1)

$$\{f, g\} := \sum_{i=1}^n \left(\frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i} \right). \quad (6)$$

Independently of the existence of a Poisson Bracket, the space \mathcal{F} is a commutative and associative algebra under the operation of pointwise multiplication:

$$(f \cdot g)(x) := f(x)g(x). \quad (7)$$

This means that the multiplication operation is also a map $\mathcal{F} \times \mathcal{F} \rightarrow \mathcal{F}$ (simply denoted by ‘ \cdot ’) which satisfies the following conditions for all $f, g, h \in \mathcal{F}$ and $\lambda \in \mathbb{R}$:

$$f \cdot g = g \cdot f \quad \text{commutativity,} \quad (8)$$

$$f \cdot (g + \lambda h) = f \cdot g + \lambda f \cdot h \quad \text{linearity,} \quad (9)$$

$$f \cdot (g \cdot h) = (f \cdot g) \cdot h \quad \text{associativity.} \quad (10)$$

The two structures are intertwined by the following condition, which expresses the fact that each map $D_f : \mathcal{F} \rightarrow \mathcal{F}, g \mapsto D_f(g) := \{f, g\}$, is a derivation of the associative algebra for each $f \in \mathcal{F}$:

$$\{f, g \cdot h\} = \{f, g\} \cdot h + g \cdot \{f, h\}. \quad (11)$$

The Jacobi identity now implies that (\circ denotes composition) $D_f \circ D_g - D_g \circ D_f = D_{\{f,g\}}$.² Taken all this together this makes \mathcal{F} into a Poisson algebra, whose abstract definition is as follows:

Definition 1. A *Poisson algebra* is a vector space V with two maps $V \times V \rightarrow V$, denoted by ‘ $\{, \}$ ’ and ‘ \cdot ’, which turn V into a Lie algebra (defined by (3-5)) and a commutative and associative algebra (defined by (8-10)) respectively, such that (11) holds.

Simply writing the symbol \mathcal{F} now becomes ambiguous since it does not indicate which of these different structures we wish to be implicitly understood. I shall use the convention to let ‘+’ indicate the vector-space structure, $(+, \{, \})$ the Lie-algebra structure, $(+, \cdot)$ the associative structure, and $(+, \{, \}, \cdot)$ the Poisson structure. To avoid confusion I will then sometimes write:

$$\mathcal{F} \quad \text{for the set ,} \quad (12)$$

$$\mathcal{F}(+, \{, \}) \quad \text{for the Lie algebra ,} \quad (13)$$

$$\mathcal{F}(+, \cdot) \quad \text{for the associative algebra ,} \quad (14)$$

$$\mathcal{F}(+, \{, \}, \cdot) \quad \text{for the Poisson algebra ,} \quad (15)$$

formed by our subset of functions from $C^\infty(P)$. Sometimes I will indicate the subset of functions by a subscript on \mathcal{F} . For example, I will mostly restrict P to be \mathbb{R}^{2n} with coordinates (q^i, p_i) . It then makes sense to restrict to functions which are polynomials in these coordinates.³ Then the following subspaces will turn out to be important in the sequel:

$$\mathcal{F}_\infty \quad : \quad C^\infty\text{-functions,} \quad (16)$$

$$\mathcal{F}_{\text{pol}} \quad : \quad \text{polynomials in } q\text{'s and } p\text{'s,} \quad (17)$$

$$\mathcal{F}_{\text{pol}(1)} \quad : \quad \text{polynomials of at most first order,} \quad (18)$$

$$\mathcal{F}_{\text{pol}(2)} \quad : \quad \text{polynomials of at most second order,} \quad (19)$$

$$\mathcal{F}_{\text{pol}(\infty,1)} \quad : \quad \text{polynomials of at most first order in the } p\text{'s} \\ \text{whose coefficients are polynomials in the } q\text{'s.} \quad (20)$$

An otherwise unrestricted polynomial dependence is clearly preserved under addition, scalar multiplication, multiplication of functions, and also taking the Poisson

²This can be expressed by saying that the assignment $f \mapsto D_f$ is a Lie homomorphism from the Lie algebra \mathcal{F} to the Lie algebra of derivations on \mathcal{F} . Note that the derivations form an associative algebra when multiplication is defined to be composition, and hence also a Lie algebra when the Lie product is defined to be the commutator.

³Recall that you need an affine structure on a space in order to give meaning to the term ‘polynomial functions’.

Bracket (6). Hence \mathcal{F}_{poi} forms a Poisson subalgebra. This is not true for the other subspaces listed above, which still form Lie subalgebras but not associative algebras.

2.2 Defining ‘canonical quantisation’

Roughly speaking, Dirac’s approach to quantisation consists in mapping certain functions on P to the set $\text{SYM}(\mathcal{H})$ of symmetric operators (sometimes called ‘formally self adjoint’) on a Hilbert space \mathcal{H} . Suppose these operators have a common invariant dense domain $\mathcal{D} \subset \mathcal{H}$ (typically the ‘Schwarz space’), then it makes sense to freely multiply them. This generates an associative algebra of operators (which clearly now also contains non-symmetric ones) defined on \mathcal{D} . Note that every associative algebra is automatically a Lie algebra by defining the Lie product proportional to the commutator (cf. Appendix 2):

$$[X, Y] := X \cdot Y - Y \cdot X. \quad (21)$$

Since the commutator of two symmetric operators is antisymmetric, we obtain a Lie-algebra structure on the real vector space of symmetric operators with invariant dense domain \mathcal{D} by defining the Lie product as imaginary multiple of the commutator; this I will write as $\frac{1}{i\hbar}[\cdot, \cdot]$ where \hbar is a real (dimensionful) constant, eventually to be identified with Planck’s constant divided by 2π .

Note that I deliberately did *not* state that classical observables should be mapped to *self adjoint* operators. Instead I only required the operators to be symmetric, which is a weaker requirement. This important distinction (see e.g. [16]) is made for the following reason (see e.g. sect. VIII in [16] for the mathematical distinction): let \hat{f} be the operator corresponding to the phase-space function f . If \hat{f} were self adjoint, then the quantum flow $U(t) = \exp(it\hat{f})$ existed for all $t \in \mathbb{R}$, even if the classical Hamiltonian vector field for f is incomplete (cf. Appendix 1) so that the classical flow does not exist for all flow parameters in \mathbb{R} . Hence self adjointness seems too strong a requirement for such f whose classical flow is incomplete (which is the generic situation). Therefore one generally only requires the operators to be symmetric and strengthens this explicitly for those f whose classical flow is complete (see below).

A first attempt to mathematically define Dirac’s quantisation strategy could now consist in the following: find a ‘suitable’ Lie homomorphism \mathcal{Q} from a ‘suitable’ Lie subalgebra $\mathcal{F}' \subset \mathcal{F}(+, \{, \})$ to the Lie algebra $\text{SYM}(\mathcal{H})$ of symmetric operators on a Hilbert space \mathcal{H} with some common dense domain $\mathcal{D} \subset \mathcal{H}$. The map \mathcal{Q} will be called the *quantisation map*. Note that this map is a priori not required in any way to preserve the associative structure, i.e. no statement is made to the effect that $\mathcal{Q}(f \cdot g) = \mathcal{Q}(f) \cdot \mathcal{Q}(g)$, or similar.

To be mathematically precise, we still need to interpret the word ‘suitable’ which occurred twice in the above statement. For this we consider the following *test case*, which at first sight appears to be sufficiently general and sufficiently precise to be able to incorporate Dirac’s ideas in a well defined manner:

1. We restrict the Lie algebra of C^∞ -Functions on P to polynomials in (q^i, p_i) , i.e. we consider $\mathcal{F}_{\text{pol}}(+, \{, \})$.
2. As Hilbert space of states, \mathcal{H} , we consider the space of square-integrable functions $\mathbb{R}^n \rightarrow \mathfrak{H}$, where \mathfrak{H} is a *finite* dimensional Hilbert space which may account for internal degrees of freedom, like spin. \mathbb{R}^n should be thought of as ‘half’ of phase space, or more precisely the configuration space coordinatised by the set $\{q^1, \dots, q^n\}$. For integration we take the Lebesgue measure $d^n q$.
3. There exists a map $\mathcal{Q} : \mathcal{F}_{\text{pol}} \rightarrow \text{SYM}(\mathcal{H}, \mathcal{D})$ into the set of symmetric operators on \mathcal{H} with common invariant dense domain \mathcal{D} . (When convenient we also write \hat{f} instead of $\mathcal{Q}(f)$.) This map has the property that whenever $f \in \mathcal{F}_{\text{pol}}$ has a complete Hamiltonian vector field the operator $\mathcal{Q}(f)$ is in fact (essentially) self adjoint.⁴

4. \mathcal{Q} is linear:

$$\mathcal{Q}(f + \lambda g) = \mathcal{Q}(f) + \lambda \mathcal{Q}(g). \quad (22)$$

5. \mathcal{Q} intertwines the Lie structure on $\mathcal{F}_{\text{pol}}(+, \{, \})$ and the Lie structure given by $\frac{1}{i\hbar}[\cdot, \cdot]$ on $\text{SYM}(\mathcal{H}, \mathcal{D})$:

$$\mathcal{Q}(\{f, g\}) = \frac{1}{i\hbar}[\mathcal{Q}(f), \mathcal{Q}(g)]. \quad (23)$$

Here \hbar is a constant whose physical dimension is that of $p \cdot q$ (i.e. an action) which accounts for the intrinsic dimension of $\{, \}$ acquired through the differentiations (cf. (6)). Note again that the imaginary unit is necessary to obtain a Lie structure on the subset of symmetric operators.

6. Let $\mathbb{1}$ also denote the constant function with value 1 on P and $\mathbb{1}$ the unit operator; then

$$\mathcal{Q}(\mathbb{1}) = \mathbb{1}. \quad (24)$$

7. The quantisation map \mathcal{Q} is consistent with Schrödinger quantisation:

$$(\mathcal{Q}(q^i)\psi)(q) = q^i\psi(q), \quad (25)$$

$$(\mathcal{Q}(p_i)\psi)(q) = -i\hbar\partial_{q^i}\psi(q). \quad (26)$$

⁴We remark that the subset of functions whose flows are complete do not form a Lie subalgebra; hence it would not make sense to just restrict to them.

One might wonder what is actually implied by the last condition and whether it is not unnecessarily restrictive. This is clarified by the theorem of *Stone* and *von Neumann* (see e.g. [1]), which says that if the $2n$ operators $\mathcal{Q}(q^i)$ and $\mathcal{Q}(p_i)$ are represented *irreducibly up to finite multiplicity* (to allow for finitely many internal quantum numbers) and satisfy the required commutation relations, then their representation is unitarily equivalent to the Schrödinger representation given above. In other words, points 2.) and 7.) above are equivalent to, and could therefore be replaced by, the following requirement:

- 7'. The $2n$ operators $\mathcal{Q}(q^i), \mathcal{Q}(p_i)$ act irreducibly up to at most finite multiplicity on \mathcal{H} .

Finally there is a technical point to be taken care of. Note that the commutator on the right hand side of (23)—and hence the whole equation—only makes sense on the subset $\mathcal{D} \subseteq \mathcal{H}$. This becomes important if one deduces from (22) and (23) that

$$\{f, g\} = 0 \Rightarrow [\mathcal{Q}(f), \mathcal{Q}(g)] = 0, \quad (27)$$

i.e. that $\mathcal{Q}(f)$ and $\mathcal{Q}(g)$ commute *on* \mathcal{D} . Suppose that the Hamiltonian vector fields of f and g are complete so that $\mathcal{Q}(f)$ and $\mathcal{Q}(g)$ are self adjoint. Then commutativity on \mathcal{D} does *not* imply that $\mathcal{Q}(f)$ and $\mathcal{Q}(g)$ commute in the usual (strong) sense of commutativity of self-adjoint operators, namely that all their spectral projectors mutually commute (compare [16], p. 271). This we pose as an extra condition:

8. If f, g have complete Hamiltonian vector fields and $\{f, g\} = 0$; then $\mathcal{Q}(f)$ commutes with $\mathcal{Q}(g)$ in the strong sense, i.e. their families of spectral projectors commute.

This extra condition will facilitate the technical presentation of the following arguments, but we remark that it can be dispensed with [8].

2.3 The theorem of Groenewold and van Howe

In a series of papers Groenewold [9] and van Hove [19, 18] showed that a canonical quantisation satisfying requirements 1.–8. does *not* exist. The proof is instructive and therefore we shall present it in detail. For logical clarity it is advantageous to divide it into two parts:

Part 1 shows the following ‘squaring laws’:

$$\mathcal{Q}(q^2) = [\mathcal{Q}(q)]^2, \quad (28)$$

$$\mathcal{Q}(p^2) = [\mathcal{Q}(p)]^2, \quad (29)$$

$$\mathcal{Q}(qp) = \frac{1}{2}[\mathcal{Q}(q)\mathcal{Q}(p) + \mathcal{Q}(p)\mathcal{Q}(q)]. \quad (30)$$

Next to elementary manipulations the proof of part 1 uses a result concerning the Lie algebra $sl(2, \mathbb{R})$, which we shall prove in Appendix 2. Note that in the canonical approach as formulated here *no* initial assumption whatsoever was made concerning the preservation of the associative structure. Points 4. and 5. only required the Lie structure to be preserved. The importance of part 1 is to show that such a partial preservation of the associative structure can actually be derived. It will appear later (cf. Sect. 2.5) that this consequence could not have been drawn without the irreducibility requirement 7').

Part 2 shows that the squaring laws lead to a contradiction to (23) on the level of higher than second-order polynomials.

Let us now turn to the proofs. To save notation we write \hat{f} instead of $\mathcal{Q}(f)$. Also, we restrict attention to $n = 1$, i.e. we have one q and one p coordinate on the two dimensional phase space \mathbb{R}^2 . In what follows, essential use is repeatedly made of condition 8 in the following form: assume $\{f, q\} = 0$ then (23) and condition 8 require that \hat{f} (strongly) commutes with \hat{q} , which in the Schrödinger representation implies that \hat{f} has the form $(\hat{f}\psi)(q) = A(q)\psi(q)$, where $A(q)$ is a Hermitean operator (matrix) in the finite dimensional (internal) Hilbert space \mathfrak{H} .

Proof of part 1 We shall present the argument in 7 small steps. Note that throughout we work in the Schrödinger representation.

- i) Calculate \hat{q}^2 : we have $\{q^2, q\} = 0$, hence $\hat{q}^2 = A(q)$. Applying (23) and (25) to $\{p, q^2\} = -2q$ gives $\frac{1}{i\hbar}[\hat{p}, \hat{q}^2] = -2\hat{q}$ and hence $A'(q) = 2q$ (here we suppress to write an explicit $\mathbb{1}$ for the unit operator in \mathfrak{H}), so that

$$\hat{q}^2 = \hat{q}^2 - 2\epsilon_-, \quad (31)$$

where ϵ_- is a constant (i.e. q independent) Hermitean matrix in \mathfrak{H} .

- ii) Calculate \hat{p}^2 : this is easily obtained by just Fourier transforming the case just done. Hence

$$\hat{p}^2 = \hat{p}^2 + 2\epsilon_+, \quad (32)$$

where ϵ_+ is a constant Hermitean matrix in \mathfrak{H} (here, as in (31), the conventional factor of 2 and the signs are chosen for later convenience).

- iii) Calculate $\hat{q}\hat{p}$: We apply (23) to $4qp = \{q^2, p^2\}$ and insert the results (31) and (32):

$$\hat{q}\hat{p} = \frac{1}{4i\hbar}[\hat{q}^2, \hat{p}^2] = \frac{1}{4i\hbar}[\hat{q}^2, \hat{p}^2] - \frac{1}{i\hbar}[\epsilon_-, \epsilon_+] = \frac{1}{2}(\hat{q}\hat{p} + \hat{p}\hat{q}) + \mathfrak{h}, \quad (33)$$

where

$$\mathfrak{h} := \frac{1}{i\hbar}[\mathfrak{e}_+, \mathfrak{e}_-]. \quad (34)$$

In the last step of (33) we iteratively used the general rule

$$[A, BC] = [A, B]C + B[A, C]. \quad (35)$$

iv) Next consider the quantities

$$h := \frac{1}{2}(\hat{q}\hat{p} + \hat{p}\hat{q}), \quad (36)$$

$$e_+ := \frac{1}{2}\hat{p}^2, \quad (37)$$

$$e_- := -\frac{1}{2}\hat{q}^2. \quad (38)$$

By straightforward iterative applications of (35) short computations yield

$$\frac{1}{i\hbar}[e_+, e_-] = h, \quad \frac{1}{i\hbar}[h, e_{\pm}] = \pm 2 e_{\pm}, \quad (39)$$

which show that e_{\pm}, h furnish a representation of the Lie algebra of $sl(2, \mathbb{R})$ of real traceless 2×2 matrices (see Appendix 2 for details).

v) On the other hand, defining

$$H := \hat{q}\hat{p}, \quad (40)$$

$$E_+ := \frac{1}{2}\hat{p}^2, \quad (41)$$

$$E_- := -\frac{1}{2}\hat{q}^2, \quad (42)$$

we can directly use (23) to calculate their Lie brackets. This shows that they also satisfy the $sl(2, \mathbb{R})$ algebra:

$$\frac{1}{i\hbar}[E_+, E_-] = H, \quad \frac{1}{i\hbar}[H, E_{\pm}] = \pm 2 E_{\pm}. \quad (43)$$

vi) Inserting into (43) the results (31) (32) (33) now implies that the Hermitean matrices $\mathfrak{e}_{\pm}, \mathfrak{h}$ too satisfy the $sl(2, \mathbb{R})$ algebra:

$$\frac{1}{i\hbar}[\mathfrak{e}_+, \mathfrak{e}_-] = \mathfrak{h}, \quad \frac{1}{i\hbar}[\mathfrak{h}, \mathfrak{e}_{\pm}] = \pm 2 \mathfrak{e}_{\pm}. \quad (44)$$

vii) Finally we invoke the following result from Appendix 2:

Lemma 1. *Let A, B_+, B_- be finite dimensional anti-Hermitean matrices which satisfy $A = [B_+, B_-]$ and $[A, B_{\pm}] = \pm 2B_{\pm}$, then $A = B_{\pm} = 0$.*

Applying this to our case by setting $A = \frac{1}{i\hbar}\mathfrak{h}$ and $B_{\pm} = \frac{1}{i\hbar}\mathfrak{e}_{\pm}$ implies

$$\mathfrak{e}_{\pm} = 0 = \mathfrak{h}. \quad (45)$$

Inserting this into (31-33) yields (28-30) respectively. This ends the proof of part 1.

Proof of part 2

Following [8], we first observe that the statements (28-30) can actually be generalised: Let P be any real polynomial, then

$$\widehat{P(q)} = P(\hat{q}), \quad (46)$$

$$\widehat{P(p)} = P(\hat{p}), \quad (47)$$

$$\widehat{P(q)p} = \frac{1}{2}(P(\hat{q})\hat{p} + \hat{p}P(\hat{q})), \quad (48)$$

$$\widehat{P(p)q} = \frac{1}{2}(P(\hat{p})\hat{q} + \hat{q}P(\hat{p})). \quad (49)$$

To complete the proof of part 2 it is sufficient to prove (46) and (47) for $P(x) = x^3$, and (48) and (49) for $P(x) = x^2$. This we shall do first. The cases for general polynomials—which we do not need—follow by induction and linearity. Again we break up the argument, this time into 5 pieces.

- i) We first note that $\{q, q^3\} = 0$ implies via (23) that \hat{q} and \hat{q}^3 commute. Since \hat{q} and \hat{q}^3 commute anyway we can write $\hat{q}^3 - \hat{q}^3 = A(q)$, where $A(q)$ takes values in the space of Hermitean operators on \mathfrak{H} .
- ii) We next show that $A(q)$ also commutes with \hat{p} . This follows from the following string of equations, where we indicated the numbers of the equations used in the individual steps as superscripts over the equality signs:

$$[\hat{q}^3, \hat{p}] \stackrel{23}{=} i\hbar\{\widehat{q^3}, p\} \stackrel{6}{=} 3i\hbar\widehat{q^2} \stackrel{28}{=} 3i\hbar\hat{q}^2 \stackrel{35}{=} [\hat{q}^3, \hat{p}]. \quad (50)$$

Hence $A(q)$ equals a q -independent matrix, \mathfrak{a} , and we have

$$\hat{q}^3 = \hat{q}^3 + \mathfrak{a}. \quad (51)$$

- iii) We show that the matrix \mathfrak{a} must actually be zero by the following string of equations:

$$\begin{aligned} \hat{q}^3 &\stackrel{6}{=} \frac{1}{3}\{\widehat{q^3}, qp\} \stackrel{23}{=} \frac{1}{3i\hbar}[\hat{q}^3, \widehat{qp}] \stackrel{30,51}{=} \frac{1}{3i\hbar}[\hat{q}^3 + \mathfrak{a}, \frac{1}{2}(\hat{q}\hat{p} + \hat{p}\hat{q})] \\ &\stackrel{*}{=} \frac{1}{6i\hbar}[\hat{q}^3, (\hat{q}\hat{p} + \hat{p}\hat{q})] \stackrel{35}{=} \hat{q}^3, \end{aligned} \quad (52)$$

where at $*$ we used that a commutes with \hat{q} and \hat{p} . This proves (46) for $P(q) = q^3$. Exchanging p and q and repeating the proof shows (47) for $P(p) = p^3$.

iv) Using what has been just shown allows to prove (48) for $P(q) = q^2$:

$$\widehat{q^2 p} \stackrel{6}{=} \frac{1}{6} \widehat{\{q^3, p^2\}} \stackrel{23}{=} \frac{1}{6i\hbar} [\widehat{q^3}, \widehat{p^2}] \stackrel{46,29}{=} \frac{1}{6i\hbar} [\hat{q}^3, \hat{p}^2] \stackrel{35}{=} \frac{1}{2} (\hat{q}^2 \hat{p} + \hat{p} \hat{q}^2). \quad (53)$$

Exchanging q and p proves (49) for $P(p) = p^2$.

v) Finally we apply the quantisation map to both sides of the classical equality

$$\frac{1}{9} \{q^3, p^3\} = \frac{1}{3} \{q^2 p, p^2 q\}. \quad (54)$$

On the left hand side we replace $\widehat{q^3}$ and $\widehat{p^3}$ with \hat{q}^3 and \hat{p}^3 respectively and then successively apply (35); this leads to

$$\hat{q}^2 \hat{p}^2 - 2i\hbar \hat{q} \hat{p} - \frac{2}{3} \hbar^2 \mathbb{1}. \quad (55)$$

On the right hand side of (54) we now use (48) and (49) to replace $\widehat{q^2 p}$ and $\widehat{p^2 q}$ with $\frac{1}{2} (\hat{q}^2 \hat{p} + \hat{p} \hat{q}^2)$ and $\frac{1}{2} (\hat{p}^2 \hat{q} + \hat{q} \hat{p}^2)$ respectively and again successively apply (35). This time we obtain

$$\hat{q}^2 \hat{p}^2 - 2i\hbar \hat{q} \hat{p} - \frac{1}{3} \hbar^2 \mathbb{1}, \quad (56)$$

which differs from (55) by a term $-\frac{1}{3} \hbar^2 \mathbb{1}$. But according to (23) both expressions should coincide, which means that we arrived at a contradiction. This completes part 2 and hence the proof of the theorem of Groenewold and van Howe.

2.4 Discussion

The GvH-Theorem shows that the Lie algebra of *all* polynomials on \mathbb{R}^{2n} cannot be quantised (and hence no Lie subalgebra of $C^\infty(P)$ containing the polynomials). But its proof has also shown that the Lie *subalgebra*

$$\mathcal{F}_{\text{pol}(2)} := \text{span} \{1, q, p, q^2, p^2, qp\} \quad (57)$$

of polynomials of at most quadratic order *can* be quantised. This is just the essence of the ‘squaring laws’ (28-30).

To see that $\mathcal{F}_{\text{pol}(2)}$ is indeed a Lie subalgebra, it is sufficient to note that the Poisson bracket (6) of a polynomial of n -th and a polynomial of m -th order is a

polynomial of order $(n+m-2)$. Moreover, it can be shown that $\mathcal{F}_{\text{pol}(2)}$ is a *maximal* Lie subalgebra of \mathcal{F}_{pol} , i.e. that there is no other proper Lie subalgebra \mathcal{F}' which properly contains $\mathcal{F}_{\text{pol}(2)}$, i.e. which satisfies $\mathcal{F}_{\text{pol}(2)} \subset \mathcal{F}' \subset \mathcal{F}_{\text{pol}}$.

$\mathcal{F}_{\text{pol}(2)}$ contains the Lie subalgebra of all polynomials of at most first order:

$$\mathcal{F}_{\text{pol}(1)} := \text{span} \{1, q, p\} . \quad (58)$$

This is clearly a Lie ideal in $\mathcal{F}_{\text{pol}(2)}$ (not in \mathcal{F}_{pol}), since Poisson brackets between quadratic and linear polynomials are linear. $\mathcal{F}_{\text{pol}(1)}$ is also called the ‘Heisenberg algebra’. According to the rules (25-26) the Heisenberg algebra was required to be represented irreducibly (cf. the discussion following (26)). What is so special about the Heisenberg algebra? First, observe that it contains enough functions to coordinatise phase space, i.e. that no two points in phase space assign the same values to the functions contained in the Heisenberg algebra. Moreover, it is a minimal subalgebra of \mathcal{F}_{pol} with this property. Hence it is a minimal set of classical observables whose values allow to uniquely fix a classical state (point in phase space). The irreducibility requirement can then be understood as saying that this property should essentially also be shared by the quantised observables, at least up to *finite* multiplicities which correspond to the ‘internal’ Hilbert space \mathfrak{H} (a ray of which is fixed by finitely many eigenvalues). We will have more to say about this irreducibility postulate below.

The primary lesson from the GvH is that $\mathcal{F}_{\text{pol}} \subset \mathcal{F}_{\infty}$ was chosen too big. It is not possible to find a quantisation map $\mathcal{Q} : \mathcal{F}_{\text{pol}}(+, \{, \}) \rightarrow \text{SYM}(\mathcal{H})$ which intertwines the Lie structures $\{, \}$ and $\frac{1}{i\hbar}[\cdot, \cdot]$. This forces us to reformulate the canonical quantisation programme. From the discussion so far one might attempt the following rules

Rule 1. Given the Poisson algebra $\mathcal{F}_{\text{pol}}(+, \{, \}, \cdot)$ of all polynomials on phase space. Find a Lie subalgebra $\mathcal{F}_{\text{irr}} \subset \mathcal{F}_{\text{pol}}(+, \{, \})$ of ‘basic observables’ which fulfills the two conditions: (1) \mathcal{F}_{irr} contains sufficiently many functions so as to coordinatise phase space, i.e. no two points coincide in all values of functions in \mathcal{F}_{irr} ; (2) \mathcal{F}_{irr} is minimal in that respect, i.e. there is no Lie subalgebra $\mathcal{F}'_{\text{irr}}$ properly contained in \mathcal{F}_{irr} which also fulfills (1).

Rule 2. Find another Lie subalgebra $\mathcal{F}_{\text{quant}} \subset \mathcal{F}_{\text{pol}}(+, \{, \})$ so that $\mathcal{F}_{\text{irr}} \subseteq \mathcal{F}_{\text{quant}}$ and that $\mathcal{F}_{\text{quant}}$ can be quantised, i.e. a Lie homomorphism $\mathcal{Q} : \mathcal{F}_{\text{quant}} \rightarrow \text{SYM}(\mathcal{H})$ can be found, which intertwines the Lie structures $\{, \}$ and $\frac{1}{i\hbar}[\cdot, \cdot]$. Require \mathcal{Q} to be such that $\mathcal{Q}(\mathcal{F}_{\text{irr}})$ act almost irreducibly, i.e. up to finite multiplicity, on \mathcal{H} . Finally, require that $\mathcal{F}_{\text{quant}}$ be maximal in \mathcal{F}_{pol} , i.e. that there is no $\mathcal{F}'_{\text{quant}}$ with $\mathcal{F}_{\text{quant}} \subset \mathcal{F}'_{\text{quant}} \subset \mathcal{F}_{\text{pol}}(+, \{, \})$.

Note that the choice of $\mathcal{F}_{\text{quant}}$ is generally far from unique. For example, instead of choosing $\mathcal{F}_{\text{quant}} = \mathcal{F}_{\text{pol}(2)}$, i.e. the polynomials of at most quadratic order,

we could choose $\mathcal{F}_{\text{quant}} = \mathcal{F}_{\text{pol}(\infty,1)}$, the polynomials of at most linear order in momenta with coefficients which are arbitrary polynomials in q . A general element in $\mathcal{F}_{\text{pol}(\infty,1)}$ has the form

$$f(q, p) = g(q) + h(q) p \quad (59)$$

where g, h are arbitrary polynomials with real coefficients. The Poisson bracket of two such functions is

$$\{f_1, f_2\} = \{g_1 + h_1 p, g_2 + h_2 p\} = g_3 + h_3 p, \quad (60)$$

where

$$g_3 = g'_1 h_2 - g'_2 h_1 \quad \text{and} \quad h_3 = h'_1 h_2 - h_1 h'_2. \quad (61)$$

The quantisation map applied to f is then given by

$$\widehat{f} = g(\hat{q}) - i\hbar\left(\frac{1}{2}h'(\hat{q}) + h(\hat{q})\frac{d}{d\hat{q}}\right), \quad (62)$$

where h' denotes the derivative of h and \hat{q} and \hat{p} are just the Schrödinger operators ‘multiplication by q ’ and ‘ $-i\hbar d/dq$ ’ respectively. The derivative term proportional to h' is necessary to make \widehat{f} symmetric (an overline denoting complex conjugation):

$$\begin{aligned} \left[\frac{i}{2}h'(q)\psi(q) + ih(q)\psi'(q)\right]\overline{\phi(q)} &= \psi(q)\overline{\left[\frac{i}{2}h'(q)\phi(q) + ih(q)\phi'(q)\right]} \\ &+ (ih\psi\overline{\phi})'(q), \end{aligned} \quad (63)$$

where the last term vanishes upon integration. Moreover, a simple computation readily shows that the map $f \mapsto \widehat{f}$ indeed defines a Lie homomorphism from $\mathcal{F}_{\text{pol}(\infty,1)}$ to $\text{SYM}(\mathcal{H})$:

$$\frac{1}{i\hbar}[\widehat{f}_1, \widehat{f}_2] = g_3(q) - i\hbar\left(\frac{1}{2}h'_3(q) + h_3(q)\frac{d}{dq}\right) = \widehat{\{f_1, f_2\}}, \quad (64)$$

with $f_{1,2}$ and g_3, h_3 as in (60) and (61) respectively. Hence (62) gives a quantisation of $\mathcal{F}_{\text{pol}(\infty,1)}$.

It can be shown ([8], Thm. 8) that $\mathcal{F}_{\text{pol}(2)}$ and $\mathcal{F}_{\text{pol}(\infty,1)}$ are the only maximal Lie subalgebras of \mathcal{F}_{pol} which contain the Heisenberg algebra $\mathcal{F}_{\text{pol}(1)}$. In this sense, if one restricts to polynomial functions, there are precisely two inextendible quantisations.

So far we restricted attention to polynomial functions. Since \mathcal{F}_{pol} is already too big to be quantised, there is clearly no hope to quantise all C^∞ functions on our phase space \mathbb{R}^{2n} . For general phase spaces P (i.e. not isomorphic to \mathbb{R}^{2n}) there is generally no notion of ‘polynomials’ and hence no simple way to characterise suitable Lie subalgebras of $\mathcal{F}_\infty(+, \{, \})$. But experience with the GvH Theorem suggests anyway to conjecture that, subject to some irreducibility postulate for some

minimal choice of $\mathcal{F}_{\text{irr}} \subset \mathcal{F}_{\infty}$, there is *never* a quantisation of \mathcal{F}_{∞} . (A quantisation of all C^{∞} functions is called *full quantisation* in the literature.) Surprisingly there is a non-trivial counterexample to this conjecture: it has been shown that a full quantisation exists for the 2-torus [6]. One might first guess that this is somehow due to the compactness of the phase space. But this is not true, as a GvH obstruction to full quantisation does exist for the 2-sphere [7]. But the case of the 2-torus seems exceptional, even mathematically. The general expectation is indeed that GvH-like obstructions are in some sense generic, though, to my knowledge, there is no generally valid formulation and corresponding theorem to that effect. (For an interesting early attempt in this direction see [5].) Hence we face the problem to determine \mathcal{F}_{irr} and $\mathcal{F}_{\text{quant}}$ within \mathcal{F}_{∞} . There is no general theory how to do this. If P is homogeneous, i.e. if there is a finite dimensional Lie group G (called the ‘canonical group’) that acts transitively on P and preserves the Poisson bracket (like the $2n$ translations in \mathbb{R}^{2n}) one may generate \mathcal{F}_{irr} from the corresponding momentum maps. This leads to a beautiful theory [12] for such homogeneous situations, but general finite dimensional P do not admit a finite dimensional canonical group G , and then things become much more complicated.

2.5 The rôle of the irreducibility-postulate

Definition 2. Quantisation without the irreducibility postulate (25-26) is called *pre-quantisation*.

Given the GvH result, the following is remarkable:

Theorem 1. *A prequantisation of the Lie algebra $\mathcal{F}_{\infty}(+, \{, \})$ of all C^{∞} -functions on \mathbb{R}^{2n} exists.*

The proof is constructive by means of *geometric quantisation*. Let us briefly recall the essentials of this approach: The Hilbert space of states is taken to be $\mathcal{H} = L^2(\mathbb{R}^{2n}, d^n q d^n p)$, i.e. the square integrable functions on *phase space* ($2n$ coordinates), instead of configuration space (n coordinates). The quantisation map is as follows⁵:

$$\mathcal{Q}(f) = i\hbar\nabla_{X_f} + f, \quad (66)$$

⁵Unlike in ordinary Schrödinger quantisation, where $|\psi(q)|^2$ is the probability density for the system in configuration space, the corresponding quantity $|\psi(q, p)|^2$ in geometric quantisation has *not* the interpretation of a probability density in phase space. The formal reason being that in geometric quantisation \hat{q} is not just a multiplication operator (cf. (72)). For example, if ψ has support in an arbitrary small neighbourhood U of phase space this does not mean that we can simultaneously reduce the uncertainties of \hat{q} and \hat{p} , since this would violate the uncertainty relations which hold unaltered in geometric quantisation. Recall that the uncertainty relations just depend on the commutation relations since they derive from the following generally valid formula by dropping the last term: $(\langle \cdot \rangle)_{\psi}$

where ∇ is a ‘covariant-derivative’ operator, which is

$$\nabla = d + A. \quad (67)$$

Here d is just the ordinary (exterior) derivative and the connection 1-form, A , is proportional to the canonical 1-form (cf. (96)) $\theta := p_i dq^i$:

$$A = -\frac{i}{\hbar} \theta = -\frac{i}{\hbar} p_i dq^i. \quad (68)$$

The curvature, $F = dA$, is then proportional to the symplectic 2-form $\omega = d\theta$:

$$F = \frac{i}{\hbar} \omega = \frac{i}{\hbar} dq^i \wedge dp_i. \quad (69)$$

If X_f is the Hamiltonian vector field on phase space associated to the phase-space function f (cf. (91)), then in canonical coordinates it has the form

$$X_f = (\partial_{p_i} f) \partial_{q^i} - (\partial_{q^i} f) \partial_{p_i}. \quad (70)$$

The map $f \mapsto X_f$ is a Lie homomorphism from $\mathcal{F}_\infty(+, \{, \})$ to the Lie algebra of vector fields on phase space, i.e. $X_{\{f, g\}} = [X_f, X_g]$. The operator \hat{f} is formally self-adjoint and well defined on Schwarz-space (rapidly decreasing functions), which we take as our invariant dense domain \mathcal{D} . Explicitly its action reads:

$$\hat{f} = i\hbar((\partial_{q^i} f) \partial_{p_i} - (\partial_{p_i} f) \partial_{q^i}) + (f - (\partial_{p_i} f) p_i), \quad (71)$$

which clearly shows that all operators are differential operators of at most degree one. This makes it obvious that a squaring-law in the form $\hat{f}\hat{g} = \widehat{fg}$ never applies. For example, for $n = 1$ we have for \hat{q}, \hat{p} and their squares:

$$\hat{q} = q + i\hbar \partial_p, \quad \widehat{q^2} = q^2 + 2i\hbar \partial_p, \quad (72)$$

$$\hat{p} = -i\hbar \partial_q, \quad \widehat{p^2} = -p^2 - 2i\hbar p \partial_q. \quad (73)$$

One now proves by direct computation that (66) indeed defines a Lie homomorphism:

$$\begin{aligned} \frac{1}{i\hbar} [\mathcal{Q}(f), \mathcal{Q}(g)] &= \frac{1}{i\hbar} [i\hbar \nabla_{X_f} + f, i\hbar \nabla_{X_g} + g] \\ &= i\hbar [\nabla_{X_f}, \nabla_{X_g}] + X_f(g) - X_g(f) \\ &= i\hbar (\nabla_{[X_f, X_g]} + F(X_f, X_g)) + 2\{f, g\} \\ &= i\hbar \nabla_{X_{\{f, g\}}} + \{f, g\} = \mathcal{Q}(\{f, g\}), \end{aligned} \quad (74)$$

denotes the expectation value in the state ψ , $[\cdot, \cdot]_+$ the anticommutator and $\hat{f}_0 := \hat{f} - \langle \hat{f} \rangle_\psi \mathbb{1}$:

$$\langle \hat{f}_0^2 \rangle_\psi \langle \hat{g}_0^2 \rangle_\psi \geq \frac{1}{4} \left\{ |\langle [\hat{f}, \hat{g}] \rangle_\psi|^2 + |\langle [\hat{f}_0, \hat{g}_0]_+ \rangle_\psi|^2 \right\}. \quad (65)$$

where we just applied the standard identity for the curvature of the covariant derivative (67): $F(X, Y) = \nabla_X \nabla_Y - \nabla_Y \nabla_X - \nabla_{[X, Y]}$ and also used $-i\hbar F(X_f, X_g) = \omega(X_f, X_g) = \{f, g\}$ (cf. (94)).

Let us now look at a simple specific example: the linear harmonic oscillator. We use units where its mass and angular frequency equal 1. The Hamiltonian function and vector field are then given by:

$$H = \frac{1}{2}(p^2 + q^2) \Rightarrow X_H = p\partial_q - q\partial_p, \quad (75)$$

whose quantisation according to (66) is

$$\hat{H} = -i\hbar(p\partial_q - q\partial_p) + \frac{1}{2}(q^2 - p^2). \quad (76)$$

Introducing polar coordinates on phase space: $q = r \cos(\varphi)$ $p = r \sin(\varphi)$, the Hamiltonian becomes

$$\hat{H} = i\hbar\partial_\varphi + \frac{r^2}{2} \cos(2\varphi). \quad (77)$$

The eigenvalue equation reads

$$\hat{H}\psi = E\psi \Leftrightarrow \partial_\varphi\psi = -\frac{i}{\hbar} \left(E - \frac{r^2}{2} \cos(2\varphi) \right) \psi, \quad (78)$$

whose solution is

$$\psi(r, \varphi) = \psi_0(r) \exp \left\{ -\frac{i}{\hbar} \left(E\varphi - \frac{r^2}{2} \sin(2\varphi) \right) \right\}, \quad (79)$$

where ψ_0 is an arbitrary function in $L^2(\mathbb{R}_+, r dr)$. Single valuedness requires

$$E = E_n = n\hbar, \quad n \in \mathbb{Z}, \quad (80)$$

with each energy eigenspace being isomorphic to the space of square-integrable functions on the positive real line with respect to the measure $r dr$:

$$\mathcal{H}_n = L^2(\mathbb{R}_+, r dr). \quad (81)$$

Hence we see that the difference to the usual Schrödinger quantisation is not simply an expected degeneracy of the energy eigenspaces which, by the way, turns out to be quite enormous, i.e. infinite dimensional for each energy level. What is much worse and perhaps less expected is the fact that the energy spectrum in prequantisation is a proper extension of that given by Schrödinger quantisation and, in distinction to the latter, that it is *unbounded from below*. This means that there is no ground state for the harmonic oscillator in prequantisation which definitely appears physically wrong. Hence there seems to be some deeper physical significance to the irreducibility postulate than just mere avoidance of degeneracies.

3 Constrained Systems

For systems with gauge redundancies⁶ the original phase space P does not directly correspond to the set of (mutually different) classical states. First of all, only a subset $\hat{P} \subset P$ will correspond to classical states of the system, i.e. the system is *constrained* to \hat{P} . Secondly, the points of \hat{P} label the states of the systems in a redundant fashion, that is, one state of the classical system is labeled by many points in \hat{P} . The set of points which label the same state form an orbit of the group of gauge transformations which acts on \hat{P} . ‘Lying in the same orbit’ defines an equivalence relation (denoted by \sim) on \hat{P} whose equivalence classes form the space $\bar{P} := \hat{P}/\sim$ which is called the *reduced phase space*. Its points now label the classical states in a faithful fashion. Note that it is a quotient-space of the sub-space \hat{P} of P and can, in general, therefore not be represented as a subspace of P .

A straightforward strategy to quantise such a system is to ‘solve’ the constraints, that is, to construct \bar{P} . One could then apply the same methods as for unconstrained systems, at least as long as \bar{P} will be a C^∞ -manifold with a symplectic structure (cf. Appendix 1).⁷ In particular, we can then consider the Poisson algebra of C^∞ -functions and proceed as for unconstrained systems.

However, in general it is analytically very difficult to explicitly do the quotient construction $\hat{P} \rightarrow \hat{P}/\sim = \bar{P}$, i.e. to solve the constraints *classically*. Dirac has outlined a strategy to implement the constraints *after* quantisation [4]. The basic mathematical reason why this is considered a simplification is seen in the fact that the whole problem is now posed in *linear* spaces, i.e. the construction of sub- and quotient spaces in the (linear) spaces of states and observables.

Dirac’s ideas have been reviewed, refined, and discussed many times in the literature; see e.g. the comprehensive textbook by Henneaux and Teitelboim [11]. Here we shall merely give a brief coordinate-free description of how to construct the right classical Poisson algebra of functions (the ‘physical observables’).

3.1 First-class constraints

Let (P, ω) be a symplectic manifold which is to be thought of as an initial phase space of some gauge system. The physical states then correspond to the points of

⁶We deliberately avoid the word ‘symmetry’ in this context, since the action of a gauge group has a completely different physical interpretation than the action of a proper symmetry; only the latter transforms states into other, physically distinguishable states. See section 6.3 in [13] for a more comprehensive discussion of this point.

⁷In passing we remark that even though P may (and generally is in applications) a cotangent bundle T^*Q for some configuration space Q , this need not be true for \bar{P} , i.e. there will be no space \bar{Q} such that $\bar{P} \cong T^*\bar{Q}$. For this reason it is important to develop quantisations strategies that apply to general symplectic manifolds.

some submanifold $\hat{P} \hookrightarrow P$. Usually \hat{P} is characterised as zero-level set of some given collection of functions, $\hat{P} = \{p \in P \mid \phi_\alpha(p) = 0, \alpha = 1, 2, \dots, \text{codim}(\hat{P})\}$, where $\text{codim}(\hat{P}) := \dim(P) - \dim(\hat{P})$ denotes the ‘codimension’ of \hat{P} in P . The ensuing formulae will then depend on the choice of ϕ_α , though the resulting theory should only depend on \hat{P} and not on its analytical characterisation. To make this point manifest we just work with the geometric data. As usual, we shall denote the tangent bundles of P and \hat{P} by TP and $T\hat{P}$ respectively. The restriction of TP to \hat{P} (which also contains vectors not tangent to \hat{P}) is given by $TP|_{\hat{P}} := \{X \in T_p P \mid p \in \hat{P}\}$. The ω -orthogonal complement of $T_p\hat{P}$ is now defined as follows:

$$T_p^\perp \hat{P} := \{X \in T_p P|_{\hat{P}} \mid \omega(X, Y) = 0, \forall Y \in T_p \hat{P}\}. \quad (82)$$

Definition 3. A submanifold $\hat{P} \hookrightarrow P$ is called *coisotropic* iff $T^\perp \hat{P} \subset T\hat{P}$.

Since ω is non degenerate we have $\dim T_p \hat{P} + \dim T_p^\perp \hat{P} = \dim T_p P$, hence $\dim T_p^\perp \hat{P} = \text{codim} \hat{P}$. This means that for coisotropic embeddings $i : \hat{P} \hookrightarrow P$ the kernel⁸ of the pulled-back symplectic form $\hat{\omega} := i^* \omega$ on \hat{P} has the maximal possible number of dimensions, namely $\text{codim} \hat{P}$.

Definition 4. A constrained system $\hat{P} \hookrightarrow P$ is said to be of *first class* iff \hat{P} is a coisotropic submanifold of (P, ω) .

From now on we consider only first class constraints.

Lemma 2. $T^\perp \hat{P} \subset TP|_{\hat{P}}$ is an integrable subbundle.

Proof. The statement is equivalent to saying that the commutator of any two $T^\perp \hat{P}$ -valued vector fields X, Y on \hat{P} is again $T^\perp \hat{P}$ -valued. Using $[X, Y] = L_X Y$ and formula (93) we have⁹ $[X, Y] \lrcorner \hat{\omega} = L_X(Y \lrcorner \hat{\omega}) - Y \lrcorner L_X \hat{\omega} = -Y \lrcorner d(X \lrcorner \hat{\omega}) = 0$, since $Y \lrcorner \hat{\omega} = 0 = X \lrcorner \hat{\omega}$ and $d\hat{\omega} = di^* \omega = i^* d\omega = 0$ due to $d\omega = 0$. \square

Definition 5. The *gauge algebra*, Gau , is defined to be the set of all functions (out of some function class \mathcal{F} , usually $C^\infty(P)$) which vanish on \hat{P} :

$$\text{Gau} := \{f \in \mathcal{F}(P) \mid f|_{\hat{P}} \equiv 0\}. \quad (83)$$

⁸The kernel (or ‘null-space’) of a bilinear form f on V is the subspace $\text{kernel}(f) := \{X \in V \mid f(X, Y) = 0, \forall Y \in V\}$.

⁹We shall use the symbol \lrcorner to denote the insertion of a vector (standing to the left of \lrcorner) into the first slot of a form (standing to the right of \lrcorner). For example, for the 2-form ω , $X \lrcorner \omega$ denotes the 1-form $\omega(X, \cdot)$.

Gau uniquely characterises the constraint surface \hat{P} in a coordinate independent fashion. In turn, this allows to characterise the constraints algebraically; Gau is in fact a Poisson algebra. To see this, first note that it is obviously an ideal of the associative algebra $\mathcal{F}(+, \cdot)$, since any pointwise product with an element in Gau also vanishes on \hat{P} . Next we show

Lemma 3. $f \in \text{Gau}$ implies that $X_f|_{\hat{P}}$ is $T^\perp \hat{P}$ -valued.

Proof. $f|_{\hat{P}} \equiv 0 \Rightarrow \text{kernel}(df|_{\hat{P}}) = \text{kernel}((X_f \lrcorner \omega)|_{\hat{P}}) \supseteq T\hat{P}$. Hence $X_f|_{\hat{P}}$ is $T^\perp \hat{P}$ -valued. \square

Now it is easy to see that Gau is also a Lie algebra, since for $f, g \in \text{Gau}$ we have

$$\{f, g\}|_{\hat{P}} = X_f(g)|_{\hat{P}} = X_f \lrcorner dg|_{\hat{P}} = X_g \lrcorner X_f \lrcorner \omega|_{\hat{P}} = 0, \quad (84)$$

where (91) and Lemma 3 was used in the last step. Hence Gau is shown to be an associative and Lie algebra, hence a Poisson algebra. But note that whereas it is an associative ideal it is not a Lie ideal. Indeed, for $f \in \text{Gau}$ and $g \in \mathcal{F}$ we have $\{f, g\}|_{\hat{P}} = X_f(g)|_{\hat{P}} \neq 0$ for those g which vary on \hat{P} in the direction of X_f .

The interpretation of Gau is that its Hamiltonian vector fields generate gauge transformations, that is, motions which do not correspond to physically existing degrees of freedom. Two points in \hat{P} which are on the same connected leaf of $T^\perp \hat{P}$ correspond to the *same* physical state. The observables for the system described by \hat{P} must therefore Poisson-commute with all functions in Gau. Hence one might expect the Poisson algebra of physical observables to be given by the quotient \mathcal{F}/Gau . However, since Gau is not a Lie ideal in \mathcal{F} the quotient is not a Lie algebra and hence not a Poisson algebra either. The way to proceed is to consider the biggest Poisson subalgebra of \mathcal{F} which contains Gau as Lie ideal and then take the quotient. Hence we make the following

Definition 6. The *Lie idealiser* of $\text{Gau} \subset \mathcal{F}$ is

$$\mathcal{I}_{\text{Gau}} := \{f \in \mathcal{F} \mid \{f, g\}|_{\hat{P}} = 0, \forall g \in \text{Gau}\}. \quad (85)$$

\mathcal{I}_{Gau} is the space of functions which, in Dirac's terminology [4], are said to *weakly* commute with all gauge functions $g \in \text{Gau}$; that is, $\{f, g\}$ is required to vanish only *after* restriction to \hat{P} .

Lemma 4. \mathcal{I}_{Gau} is a Poisson subalgebra of \mathcal{F} which contains Gau as ideal.

Proof. Let $f, g \in \mathcal{I}_{\text{Gau}}$ and $h \in \text{Gau}$. Then clearly $f + g \in \mathcal{I}_{\text{Gau}}$ and also $\{f \cdot g, h\}|_{\hat{P}} = f \cdot \{g, h\}|_{\hat{P}} + g \cdot \{f, h\}|_{\hat{P}} = 0$ (since each term vanishes), hence \mathcal{I}_{Gau} is

an associative subalgebra. Moreover, using the Jacobi identity, we have

$$\{\{f, g\}, h\}|_{\hat{P}} = \underbrace{\{\{h, g\}, f\}|_{\hat{P}}}_{\in \text{Gau}} + \underbrace{\{\{f, h\}, g\}|_{\hat{P}}}_{\in \text{Gau}} = 0, \quad (86)$$

which establishes that \mathcal{I}_{Gau} is also a Lie subalgebra. Gau is obviously an associative ideal in \mathcal{I}_{Gau} (since it is such an ideal in \mathcal{F}) and, by definition, also a Lie ideal. Hence it is a Poisson ideal. \square

It follows from its very definition that \mathcal{I}_{Gau} is maximal in the sense that there is no strictly larger subalgebra in \mathcal{F} in which Gau is a Poisson algebra. Now we can define the algebra of *physical observables*:

Definition 7. The *Poisson algebra of physical observables* is given by

$$\mathcal{O}_{\text{phys}} := \mathcal{I}_{\text{Gau}}/\text{Gau}. \quad (87)$$

Since the restriction to \hat{P} of a Hamiltonian vector field X_g is tangent to \hat{P} if $g \in \text{Gau}$ (by Lemma 3 and coisotropy), we have

$$\begin{aligned} \mathcal{I}_{\text{Gau}} &= \{f \in \mathcal{F} \mid X_g(f)|_{\hat{P}} = 0, \forall g \in \text{Gau}\} \\ &= \{f \in \mathcal{F} \mid X_g|_{\hat{P}}(f|_{\hat{P}}) = 0, \forall g \in \text{Gau}\}, \end{aligned} \quad (88)$$

which shows that \mathcal{I}_{Gau} is the subspace of all functions in \mathcal{F} whose restrictions to \hat{P} are constant on each connected leaf of the foliation tangent to the integrable subbundle $T^\perp \hat{P}$. If the space of leaves is a smooth manifold¹⁰ it has a natural symplectic structure. In this case it is called the *reduced phase space* $(\bar{P}, \bar{\omega})$. $\mathcal{O}_{\text{phys}}$ can then be naturally identified with the Poisson algebra of (say C^∞ -) functions thereon.

We finally mention that instead of the Lie idealiser \mathcal{I}_{Gau} we could not have taken the Lie centraliser

$$\begin{aligned} \mathcal{C}_{\text{Gau}} &:= \{f \in \mathcal{F} \mid \{f, g\} = 0, \forall g \in \text{Gau}\} \\ &= \{f \in \mathcal{F} \mid X_g(f) = 0, \forall g \in \text{Gau}\}, \end{aligned} \quad (89)$$

which corresponds to the space of functions which, in Dirac's terminology [4], *strongly* commute with all gauge functions. This space is generally far too small, as can be seen from the following

¹⁰The 'space of leaves' is the quotient space with respect to the equivalence relation 'lying on the same leaf'. If the leaves are the orbits of a group action (the group of gauge transformations) then this quotient will be a smooth manifold if the group action is smooth, proper, and free (cf. Sect. 4.1 of [1]).

Lemma 5. *If \hat{P} is a closed subset of P we have*

$$\text{Span}\{X_g(p), g \in \text{Gau}\} = \begin{cases} T_p^\perp \hat{P} & \text{for } p \in \hat{P} \\ T_p P & \text{for } p \in P - \hat{P}. \end{cases} \quad (90)$$

Proof. For $p \in \hat{P}$ we know from Lemma 3 that $X_g(p) \in T_p^\perp \hat{P}$. Locally we can always find $\text{codim}(\hat{P})$ functions $g_i \in \text{Gau}$ whose differentials dg_i (and hence whose vector fields X_{g_i}) at p are linearly independent. To see that the $X_g(p)$ span all of $T_p P$ for $p \notin \hat{P}$, we choose a neighbourhood U of p such that $U \cap \hat{P} = \emptyset$ (such U exists since $\hat{P} \subset P$ is closed by hypothesis) and $\beta \in C^\infty(P)$ such that $\beta|_U \equiv 1$ and $\beta|_{\hat{P}} \equiv 0$. Then $\beta \cdot h \in \text{Gau}$ for all $h \in C^\infty(P)$ and $(\beta \cdot h)|_U = h|_U$, which shows that $\text{Span}\{X_g(p), g \in \text{Gau}\} = \text{Span}\{X_g(p), g \in C^\infty(P)\} = T_p P$. \square

This Lemma immediately implies that functions which strongly commute with all gauge functions must have altogether vanishing directional derivatives outside \hat{P} , that is, they must be constant on any connected set outside \hat{P} . By continuity they must be also constant on any connected subset of \hat{P} . Hence the condition of strong commutativity is far too restrictive.

Sometimes strong commutativity is required, but only with a somehow preferred subset ϕ_α , $\alpha = 1, \dots, \text{codim}(\hat{P})$, of functions in Gau ; for example, the component functions of a momentum map (cf. Sect. 4.2 of [1]) of a group (the group of gauge transformations) that acts symplectomorphically (i.e. ω -preserving) on P . The size of the space of functions on P that strongly commute with all ϕ_α will generally depend delicately on the behaviour of the ϕ_α off the constraint surface, and may again turn out to be too small. The point being that even though the leaves generated by the ϕ_α may behave well *within* the zero-level set of all ϕ_α (the constraint surface), so that sufficiently many invariant (i.e. constant along the leaves) functions exist on the constraint surface, the leaves may become more ‘wild’ in infinitesimal neighbouring level sets, thereby forbidding most of these functions to be extended to some invariant functions in a neighbourhood of \hat{P} in P . See Sect. 3 of [2] for an example and more discussion of this point.

Appendix 1: Geometry of Hamiltonian Systems

A *symplectic manifold* is a pair (P, ω) , where P is a differentiable manifold and ω is a closed (i.e. $d\omega = 0$) 2-form which is non-degenerate (i.e. $\omega_p(X_p, Y_p) = 0, \forall X_p \in T_p P$, implies $Y_p = 0$ for all $p \in P$). The last condition implies that P is even dimensional. Let $C^\infty(P)$ denote the set of infinitely differentiable, real valued functions on P and $\mathcal{X}(P)$ the set of infinitely differentiable vector fields on P . $\mathcal{X}(P)$ is a real Lie algebra (cf. Appendix 2) whose Lie product is the commutator

of vector fields. There is a map $X : C^\infty(P) \rightarrow \mathcal{X}(P)$, $f \mapsto X_f$, uniquely defined by¹¹

$$X_f \lrcorner \omega = -df. \quad (91)$$

The kernel of X in $C^\infty(P)$ are the constant functions and the image of X in $\mathcal{X}(P)$ are called Hamiltonian vector fields. The Lie derivative of ω with respect to an Hamiltonian vector field is always zero:

$$L_{X_f} \omega = d(X_f \lrcorner \omega) = -ddf = 0, \quad (92)$$

where we used the following identity for the Lie derivative L_Z with respect to any vector field Z on forms of any degree:

$$L_Z = d \circ (Z \lrcorner) + (Z \lrcorner) \circ d. \quad (93)$$

The map X can be used to turn C^∞ into a Lie algebra. The Lie product $\{\cdot, \cdot\}$ on C^∞ is called Poisson bracket and defined by

$$\{f, g\} := \omega(X_f, X_g) = X_f(g) = -X_g(f), \quad (94)$$

where the 2nd and 3rd equality follows from (91). With respect to this structure the map X is a homomorphism of Lie algebras:

$$\begin{aligned} X_{\{f,g\}} \lrcorner \omega &= -d\{f,g\} \stackrel{94}{=} -d(X_g \lrcorner X_f \lrcorner \omega) \\ &\stackrel{93,91}{=} -L_{X_g}(X_f \lrcorner \omega) \\ &\stackrel{92}{=} [X_f, X_g] \lrcorner \omega. \end{aligned} \quad (95)$$

One may say that the map X has pulled back the Lie structure from $\mathcal{X}(P)$ to $C^\infty(P)$. Note that (95) also expresses the fact that Hamiltonian vector fields form a Lie subalgebra of $\mathcal{X}(P)$

Special symplectic manifolds are the cotangent bundles. Let M be a manifold and $P = T^*M$ its cotangent bundle with projection $\pi : T^*M \rightarrow M$. On P there exists a naturally given 1-form field (i.e. section of $T^*P = T^*T^*M$), called the canonical 1-form (field) θ :

$$\theta_p := p \circ \pi_*|_p. \quad (96)$$

In words, application of θ to $Z_p \in T_pP$ is as follows: project Z_p by the differential π_* , evaluated at p , into T_xM , where $x = \pi(p)$, and then act upon it by p , where $p \in \pi^{-1}(x) = T_x^*M$ is understood as 1-form on M . The exterior differential of

¹¹For notation recall footnote 9.

the canonical 1-form defines a symplectic structure on P (the minus sign being conventional):

$$\omega := -d\theta. \quad (97)$$

In canonical (Darboux-) coordinates ($\{q^i\}$ on M and $\{p_i\}$ on the fibres $\pi^{-1}(x)$) one has

$$\theta = p_i dq^i \quad \text{and} \quad \omega = dq^i \wedge dp_i, \quad (98)$$

so that

$$\{f, g\} = \sum_i \left(\frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i} \right). \quad (99)$$

In this coordinates the Hamiltonian vector field X_f reads:

$$X_f = (\partial_{p_i} f) \partial_{q^i} - (\partial_{q^i} f) \partial_{p_i}. \quad (100)$$

It is important to note that Hamiltonian vector fields need not be complete, that is, their flow need not exist for all flow parameters $t \in \mathbb{R}$. For example, consider $P = \mathbb{R}^2$ in canonical coordinates. The flow map $\mathbb{R} \times P \rightarrow P$ is then given by $(t, (q_0, p_0)) \mapsto (q(t; q_0, p_0), p(t; q_0, p_0))$, where the functions on the right hand side follow through integration of $X_f = \dot{q}(t) \partial_q + \dot{p}(t) \partial_p$, i.e.

$$\dot{q}(t) = (\partial_p f)(q(t), p(t)) \quad \text{and} \quad \dot{p}(t) = -(\partial_q f)(q(t), p(t)), \quad (101)$$

with initial conditions $q(0) = q_0, p(0) = p_0$. As simple exercises one readily solves for the flows of $f(q, p) = h(q)$, $f(q, p) = h(p)$, where $h : P \rightarrow \mathbb{R}$ is some C^1 -function, or for the flow of $f(q, p) = qp$. All these are complete. But already for $f(q, p) = q^2 p$ we obtain

$$q(t; q_0, p_0) = \frac{q_0}{1 - q_0 t} \quad \text{and} \quad p(t; q_0, p_0) = p_0 (1 - q_0 t)^2, \quad (102)$$

which (starting from $t = 0$) exists only for $t < 1/q_0$ when $q_0 > 0$ and only for $t > 1/q_0$ when $q_0 < 0$.

Appendix 2: The Lie algebra of $sl(2, \mathbb{R})$ and the absence of non-trivial, finite-dimensional representations by anti-unitary matrices

Let us first recall the definition of a Lie algebra:

Definition 8. A Lie algebra over \mathbb{F} (here standing for \mathbb{R} or \mathbb{C}) is a vector-space, L , over \mathbb{F} together with a map $V \times V \rightarrow V$, called *Lie bracket* and denoted by $[\cdot, \cdot]$, such that the following conditions hold for all $X, Y, Z \in L$ and $a \in \mathbb{F}$:

$$[X, Y] = -[Y, X] \quad \text{antisymmetry ,} \quad (103)$$

$$[X, Y + aZ] = [X, Y] + a[X, Z] \quad \text{linearity ,} \quad (104)$$

$$[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0 \quad \text{Jacobi identity .} \quad (105)$$

Note that (103) and (104) together imply linearity also in the first entry. Any associative algebra (with multiplication ‘ \cdot ’) is automatically a Lie algebra by defining the Lie bracket to be the commutator $[X, Y] := X \cdot Y - Y \cdot X$ (associativity then implies the Jacobi identity). Important examples are Lie algebras of square matrices, whose associative product is just matrix multiplication.

A sub vector-space $L' \subseteq L$ is a *sub Lie-algebra*, iff $[X, Y] \in L'$ for all $X, Y \in L'$. A sub Lie-algebra is an *ideal*, iff $[X, Y] \in L'$ for all $X \in L'$ and all $Y \in L$ (sic!). Two ideals always exist: L itself and $\{0\}$; they are called the trivial ideals. A Lie algebra is called *simple*, iff it contains only the trivial ideals. A map $\phi : L \rightarrow L'$ between Lie algebras is a *Lie homomorphism*, iff it is linear and satisfies $\phi([X, Y]) = [\phi(X), \phi(Y)]$ for all $X, Y \in L$. Note that we committed some abuse of notation by denoting the (different) Lie brackets in L and L' by the same symbol $[\cdot, \cdot]$. The kernel of a Lie homomorphism ϕ is defined by $\text{kernel}(\phi) := \{X \in L \mid \phi(X) = 0\}$ and obviously an ideal in L .

The Lie algebra denoted by $sl(2, \mathbb{F})$ is defined by the vector space of traceless 2×2 - matrices with entries in \mathbb{F} . A basis is given by

$$H = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad E_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad E_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (106)$$

Its commutation relations are:

$$[H, E_+] = 2E_+, \quad (107)$$

$$[H, E_-] = -2E_-, \quad (108)$$

$$[E_+, E_-] = H. \quad (109)$$

The first thing we prove is that $sl(2, \mathbb{F})$ is simple. For this, suppose $X = aE_+ + bE_- + cH$ is a member of an ideal $I \subseteq sl(2, \mathbb{F})$. From (107-109) we calculate

$$[E_+, [E_+, X]] = -2bE_+, \quad (110)$$

$$[E_-, [E_-, X]] = -2aE_-. \quad (111)$$

Suppose first $b \neq 0$, then (110) shows that $E_+ \in I$. Then (109) implies $H \in I$, which in turn implies through (108) that $E_- \in I$ and hence that $I = L$. Similarly one concludes for $a \neq 0$ that $I = L$. Finally assume $a = b = 0$ and $c \neq 0$ so that $H \in I$. Then (107) and (108) show that E_+ and E_- are in I , so again $I = L$. Hence we have shown that $I = L$ or $I = \{0\}$ are the only ideals.

Next consider the Lie algebra $u(n)$ of anti-Hermitian $n \times n$ matrices. It is the Lie algebra of the group $U(n)$ of unitary $n \times n$ matrices. If the group $SL(2, \mathbb{F})$ had a finite-dimensional unitary representation, i.e. if a group homomorphism $D : SL(2, \mathbb{F}) \rightarrow U(n)$ existed for some n , then we would also have a Lie homomorphism $D_* : sl(2, \mathbb{F}) \rightarrow u(n)$ by simply taking the derivative of the map D at e (= identity of $SL(2, \mathbb{F})$). We will now show that, for any integer $n \geq 1$, any Lie homomorphism $\phi : sl(2, \mathbb{F}) \rightarrow u(n)$ is necessarily the constant map onto $0 \in u(n)$. In other words, non-trivial Lie homomorphism from $sl(2, \mathbb{F})$ to $u(n)$ do not exist. On the level of groups this implies that non-trivial (i.e. not mapping everything into the identity), finite dimensional, unitary representations of $SL(2, \mathbb{F})$ do not exist. Note that for $\mathbb{F} = \mathbb{R}$ and $\mathbb{F} = \mathbb{C}$ these are (the double covers of) the proper orthochronous Lorentz groups in 2+1 and 3+1 dimensions respectively.

To prove this result, assume $T : sl(2, \mathbb{F}) \rightarrow u(n)$ is a Lie homomorphism. To save notation we write $T(H) =: A$ and $T(E_{\pm}) =: B_{\pm}$. Since T is a Lie homomorphism we have $[A, B_+] = 2B_+$, which implies

$$\text{trace}(B_+^2) = \frac{1}{2} \text{trace}(B_+(AB_+ - B_+A)) = 0, \quad (112)$$

where in the last step we used the cyclic property of the trace. But B_+ is anti Hermitian, hence diagonalisable with purely imaginary eigenvalues $\{i\lambda_1, \dots, i\lambda_n\}$ with $\lambda_i \in \mathbb{R}$. The trace on the left side of (112) is then $-\sum_i \lambda_i^2$, which is zero iff $\lambda_i = 0$ for all i , i.e. iff $B_+ = 0$. Hence $E_+ \in \text{kernel}(T)$, which in turn implies $\text{kernel}(T) = sl(2, \mathbb{F})$ since the kernel—being an ideal—is either $\{0\}$ or all of $sl(2, \mathbb{F})$ by simplicity. This proves the claim, which is stated as Lemma 1 of the main text

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