Metric approach to quantum constraints

2009 J. Phys. A: Math. Theor. 42 295303

(http://iopscience.iop.org/1751-8121/42/29/295303)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 295303 (12pp) doi:10.1088/1751-8113/42/29/295303

Metric approach to quantum constraints

Dorje C Brody[1], **Anna C T Gustavsson**[2] **and Lane P Hughston**[1]

[1] Department of Mathematics, Imperial College London, London SW7 2AZ, UK
[2] Blackett Laboratory, Imperial College London, London SW7 2AZ, UK

Received 29 April 2009, in final form 10 June 2009
Published 6 July 2009
Online at stacks.iop.org/JPhysA/42/295303

Abstract

A framework for deriving equations of motion for constrained quantum systems is introduced and a procedure for its implementation is outlined. In special cases, the proposed new method, which takes advantage of the fact that the space of pure states in quantum mechanics has both a symplectic structure and a metric structure, reduces to a quantum analogue of the Dirac theory of constraints in classical mechanics. Explicit examples involving spin-$\frac{1}{2}$ particles are worked out in detail: in the first example, our approach coincides with a quantum version of the Dirac formalism, while the second example illustrates how a situation that cannot be treated by Dirac's approach can nevertheless be dealt with in the present scheme.

PACS numbers: 03.65.Ca, 02.40.Yy

1. Introduction

Recently, there has been renewed interest in understanding the properties of constrained quantum dynamics [1–4]. The key idea behind quantum constraints is the fact that the space of pure states (rays through the origin of Hilbert space) is a symplectic manifold, and hence that Dirac's theory of constraints [5, 6] in classical mechanics is applicable in the quantum regime. The quantum state space is also equipped with a metric structure—generally absent in a classical phase space—induced by the probabilistic features of quantum mechanics. In the context of analysing constrained quantum motions it is therefore natural to examine the theory from the viewpoint of metric geometry, as opposed to a treatment based entirely on symplectic geometry. This is the goal of the present paper, which extends our earlier work [4] on the symplectic approach to quantum constraints.

The metric approach that we propose is not merely a reformulation of the Dirac formalism using the quantum symplectic structure. Indeed, there are two distinct advantages in the metric approach over the symplectic approach: (a) the metric approach to quantum constraints is generally speaking more straightforward to implement, even in situations where the constraints can be treated by the symplectic method; and (b) there are nontrivial examples of constraints that cannot be implemented in the symplectic approach but can be implemented in the metric approach. Our plan is first to outline the general metric approach to quantum constraints, and then to consider specific examples. We also derive a necessary condition for the metric approach to be equivalent to the symplectic formalism. The first example that we consider concerns the system consisting of a pair of spin-$\frac{1}{2}$ particles. We impose the constraint that the state should lie on the product subspace upon which all the energy eigenstates lie. This is the example considered in [1, 4] using the symplectic approach. Here we analyse the problem using the metric approach and show that the constrained equations of motion reduce to those obtained in [4]. The second example concerns a single spin-$\frac{1}{2}$ particle, and we impose the constraint that an observable that does not commute with the Hamiltonian must be conserved. This is perhaps the simplest example of a quantum constraint that is not evidently tractable in the symplectic approach but nevertheless can be readily dealt with by use of the metric approach.

2. Geometry of quantum state space

We begin by remarking that the space of pure quantum states associated with a Hilbert space of dimension n is the projective Hilbert space $\mathcal{P}^{n-1}$ of dimension $n-1$ (see [7–11] and references therein). We regard $\mathcal{P}^{n-1}$ as a real even-dimensional manifold Γ, and denote a typical point in Γ, corresponding to a ray in the associated Hilbert space, by $\{x^a\}_{a=1,2,\ldots,2n-2}$. It is well known that Γ has an integrable complex structure. Since the complex structure of Γ plays an important role in what follows, it may be helpful if we make a few general remarks about the relevant ideas.

We recall that an even-dimensional real manifold $\mathfrak{M}$ is said to have an almost complex structure if there exists a global tensor field J^a_b satisfying

$$J^a_c J^c_b = -\delta^a_b. \tag{1}$$

The almost complex structure is then said to be integrable if the Nijenhuis tensor

$$N^c_{ab} = J^c_d \nabla_{[a} J^d_{b]} - J^d_{[a} \nabla_{|d|} J^c_{b]} \tag{2}$$

vanishes [12]. It is straightforward to check that N^c_{ab} is independent of the choice of symmetric connection ∇_a on $\mathfrak{M}$. The vanishing of N^c_{ab} can be interpreted as follows. A complex vector field on $\mathfrak{M}$ is said to be of positive (resp., negative) type if $J^a_b V^b = +\mathrm{i}V^a$ (resp., $J^a_b V^b = -\mathrm{i}V^a$). The vanishing of N^c_{ab} is a necessary and sufficient condition for the commutator of two vector fields of the same type to be of that type.

A Riemannian metric g_{ab} on $\mathfrak{M}$ is said to be compatible with an almost complex structure J^a_b if the following conditions hold: (i) the metric is Hermitian so that

$$J^a_c J^b_d g_{ab} = g_{cd}, \tag{3}$$

and (ii) the almost complex structure is covariantly constant:

$$\nabla_a J^b_c = 0, \tag{4}$$

where ∇_a is the torsion-free Riemannian connection associated with g_{ab}. An alternative expression for the Hermitian condition is that $\Omega_{ab} = -\Omega_{ba}$, where

$$\Omega_{ab} = J^c_a g_{bc}. \tag{5}$$

It follows that $\nabla_a J^b_c = 0$ if and only if $\nabla_a \Omega_{bc} = 0$. However, if the almost complex structure is integrable, then a sufficient condition for $\nabla_a J^b_c = 0$ is $\nabla_{[a}\Omega_{bc]} = 0$. This follows on account of the identity

$$\nabla_a \Omega_{bc} = \tfrac{3}{2} J^p_b J^q_c \nabla_{[a}\Omega_{pq]} - \tfrac{3}{2}\nabla_{[a}\Omega_{bc]} + \tfrac{1}{4}\Omega_{ad} N^d_{bc}. \tag{6}$$

A manifold $\mathfrak{M}$ with an integrable complex structure and a compatible Riemannian structure is called a Kähler manifold. The antisymmetric tensor Ω_{ab} is then referred to as the 'fundamental two-form' or Kähler two-form. It follows from the definition of Ω_{ab} along with the Hermitian condition on g_{ab} that Ω_{ab} itself is Hermitian in the sense that

$$J_c^a J_d^b \Omega_{ab} = \Omega_{cd}. \tag{7}$$

Furthermore, we find that the tensor Ω^{ab} defined by

$$\Omega^{ab} = g^{ac} g^{db} \Omega_{cd} \tag{8}$$

acts as an inverse to Ω_{ab}. In particular, we have

$$\Omega^{ac} \Omega_{bc} = \delta_b^a. \tag{9}$$

In the case of quantum theory there is a natural Riemannian structure on the manifold Γ, called the Fubini–Study metric. If x and y represent a pair of points in Γ, and $|\psi(x)\rangle$ and $|\psi(y)\rangle$ are representative Hilbert space vectors, then the Fubini–Study distance between x and y is given by θ, where

$$\frac{\langle\psi(y)|\psi(x)\rangle\langle\psi(x)|\psi(y)\rangle}{\langle\psi(x)|\psi(x)\rangle\langle\psi(y)|\psi(y)\rangle} = \frac{1}{2}(1 + \cos\theta). \tag{10}$$

The Kähler form Ω_{ab} can be used to define a one-parameter family of symplectic structures on Γ, given by $\kappa\Omega_{ab}$, where κ is a nonvanishing real constant. In quantum mechanics, the symplectic structure defined by

$$\omega_{ab} = \tfrac{1}{2}\Omega_{ab} \tag{11}$$

plays a special role. In particular, if we define the inverse symplectic structure by $\omega^{ab} = 2\Omega^{ab}$ so that $\omega^{ac}\omega_{bc} = \delta_b^a$, and if we choose units such that $\hbar = 1$, then we find that the Schrödinger trajectories on Γ are given by Hamiltonian vector fields of the form

$$\dot{x}^a = \omega^{ab} \nabla_b H, \tag{12}$$

where

$$H(x) = \frac{\langle\psi(x)|\hat{H}|\psi(x)\rangle}{\langle\psi(x)|\psi(x)\rangle}. \tag{13}$$

Thus we see that the expectation of the Hamiltonian operator $\hat{H}$ gives rise to a real function $H(x)$ on Γ. This function plays the role of the Hamiltonian in the determination of the symplectic flow associated with the Schrödinger trajectory.

3. Metric formalism for quantum constraints

With these geometric tools in hand we now proceed to formulate the metric approach to quantum constraints. We consider a quantum system for which the states are subject to a family of N constraints of the form

$$\Phi^i(x) = 0, \tag{14}$$

where $i = 1, \ldots, N$. For each value of i the condition $\Phi^i(x) = 0$ defines a hypersurface in Γ. The intersection of the N hypersurfaces thus defined thereby determines the constraint surface $\mathcal{K} \in \Gamma$ within which the motion of the state is to be restricted. From a mathematical perspective, it is most natural to consider the case where the constraint surface $\mathcal{K}$ is a manifold of codimension N in Γ; but there are also situations arising in a physical context in which it seems appropriate to allow for the possibility that $\mathcal{K}$ is singular, and we shall examine some aspects of that case as well.

In the situation where $\mathcal{K}$ is nonsingular and is of codimension N, we require that the N vector fields given by $\nabla_a\Phi^i$ for $i = 1, \ldots, N$ are nonvanishing when restricted to $\mathcal{K}$, and are linearly independent at each point of $\mathcal{K}$. The tangent plane to $\mathcal{K}$ at a given point x in $\mathcal{K}$ is then spanned by a system of $2n - 2 - N$ linearly independent vectors in the tangent space of Γ at the point x with the property that they are each orthogonal to the N gradient vectors $\nabla_a\Phi^i$ at that point.

To enforce the constraints in the metric approach, we assume that the initial state of the system lies in $\mathcal{K}$, and that the modified dynamics of the quantum state trajectory are such that they can be obtained from the original Hamiltonian equations of motion if we remove from the tangent vector $\dot{x}^a$ those components that are normal to the constraint surface. It should be evident that under these assumptions the equations of motion then take the form

$$\dot{x}^a = \omega^{ab}\nabla_b H - \lambda_i g^{ab}\nabla_b\Phi^i, \tag{15}$$

where ω^{ab} is the inverse quantum symplectic structure and where the scalars $\{\lambda_i(x)\}_{i=1,\ldots,N}$ constitute a set of Lagrange multipliers. Here we have introduced for convenience the use of the summation convention for the lowercase roman 'constraint' indices. In order to determine $\{\lambda_i\}$ we consider the condition $\dot{\Phi}^j = 0$ that must hold at each point along the trajectory if the trajectory is to remain in $\mathcal{K}$. By use of the chain rule this condition can be expressed in the form

$$\dot{x}^a\nabla_a\Phi^j = 0. \tag{16}$$

Substitution of (15) into (16) then gives

$$\omega^{ab}\nabla_a\Phi^j\nabla_b H - \lambda_i g^{ab}\nabla_a\Phi^j\nabla_b\Phi^i = 0. \tag{17}$$

To simplify (17) let us define a symmetric matrix M^{ij} by setting

$$M^{ij} = g^{ab}\nabla_a\Phi^i\nabla_b\Phi^j. \tag{18}$$

We observe that if $\mathcal{K}$ is nonsingular and of codimension N, then M^{ij} has a nonvanishing determinant at each point of $\mathcal{K}$. For suppose that at some point x of $\mathcal{K}$ the determinant of M^{ij} vanished: then there would exist a null eigenvector ξ_i such that $M^{ij}\xi_i = 0$ at x. But that would imply $M^{ij}\xi_i\xi_j = 0$ at x and hence $\xi_i\nabla_a\Phi^i = 0$, which contradicts the assumption that the N gradient vectors $\nabla_a\Phi^i$ are linearly independent at each point of $\mathcal{K}$. If the matrix M^{ij} is nonsingular, we write M_{ij} for its inverse. Then $M_{ik}M^{kj} = \delta_i^j$ and we can solve (17) for λ_i to find

$$\lambda_i = M_{ij}\omega^{ab}\nabla_a\Phi^j\nabla_b H. \tag{19}$$

Substituting this expression for λ_i back into (15) we find after some rearrangement that the constrained equations of motion are given by the following modified dynamics:

$$\dot{x}^a = \omega^{ab}\nabla_b H - g^{ab}\nabla_b\Phi^i\nabla_c\Phi^j M_{ij}\omega^{cd}\nabla_d H. \tag{20}$$

These are the nonlinear equations of motion satisfied by a quantum system constrained to a nonsingular submanifold of the quantum state space.

As we remarked above, there are situations of interest where it is natural to consider the possibility that $\mathcal{K}$ might be singular. In that case, the analysis above remains valid at least locally on $\mathcal{K}$ if the initial state of the system is a nonsingular point of $\mathcal{K}$. An important example arises when the constraints are associated with quantum observables. In particular, let the constraint hypersurfaces be given by the level surfaces of the expectation values of a set of quantum observables. Thus for each value of i we have an observable $\hat{\Phi}^i$ such that $\Phi^i(x)$ is given by the expectation of the observable $\hat{\Phi}^i$ in the pure state corresponding to the point x in Γ.

The analysis of the singularities that can arise in such a system is rather delicate and is of great interest. In the case $N = 1$, the constraint is given by the requirement that the system should remain on the surface defined by the vanishing of the expectation of a single quantum observable. In general, if such a surface is of dimension 1 then it is nonsingular; but if the observable admits an eigenstate with a null eigenvalue, then that state corresponds to a singular point of the constraint surface. More generally, when N is greater than 1, M^{ij} for each i, j represents the quantum covariance between the observables $\hat{\Phi}^i$ and $\hat{\Phi}^j$ in the state represented by the point x; that is to say:

$$M^{ij} = \langle\hat{\Phi}^i\hat{\Phi}^j\rangle - \langle\hat{\Phi}^i\rangle\langle\hat{\Phi}^j\rangle. \tag{21}$$

In the case of a pair of observables, say, $\hat{\Phi}^1 = \hat{A}$ and $\hat{\Phi}^2 = \hat{B}$, we have

$$M^{ij} = \begin{pmatrix} \mathrm{var}(\hat{A}) & \mathrm{cov}(\hat{A}, \hat{B}) \\ \mathrm{cov}(\hat{A}, \hat{B}) & \mathrm{var}(\hat{B}) \end{pmatrix}. \tag{22}$$

The determinant Δ of M^{ij} is thus given by

$$\Delta = \mathrm{var}(\hat{A})\,\mathrm{var}(\hat{B}) - (\mathrm{cov}(\hat{A}, \hat{B}))^2. \tag{23}$$

It is then an exercise to show that Δ vanishes only at states that are null eigenstates of some linear combination of $\hat{A}$ and $\hat{B}$. Thus even if neither of the surfaces $A(x) = 0$ and $B(x) = 0$ are singular at the points of their intersection, the intersection itself may be singular at an isolated point. In what follows, we shall mainly be looking at the behaviour of solutions to the constraint equations away from such singular points.

4. Equivalence of metric and symplectic approaches

Before considering specific examples of constrained systems that can be described using the present approach, it will be of interest to ask how this framework might be related to the approach of Dirac [5, 6], or more precisely, its quantum counterpart [1, 2, 4] which we shall refer to as the symplectic approach. In the symplectic approach, the constrained equations of motion can be expressed in the same form as (12), but with a modified inverse symplectic structure $\tilde{\omega}^{ab}$ in place of ω^{ab}, which in effect is the induced symplectic form on the constraint surface [4]. Thus, we would like to know under what condition the metric approach leading to the right-hand side of (20) also reduces to a modified symplectic flow of the form $\tilde{\omega}^{ab}\nabla_b H$, where H is the same Hamiltonian as the one in the original Schrödinger equation (12).

Intuitively, we would expect that when there is an even number of constraints, the two methods might become equivalent. In what follows we shall establish a sufficient condition under which the symplectic approach and the metric approach are equivalent.

In order to investigate whether (20) can be rewritten in the form

$$\dot{x}^a = \tilde{\omega}^{ab}\nabla_b H \tag{24}$$

for a suitably defined antisymmetric tensor $\tilde{\omega}^{ab}$, we rearrange terms in (20) to write

$$\begin{aligned}\dot{x}^a &= (\omega^{ad} - M_{ij}g^{ab}\nabla_b\Phi^i\omega^{cd}\nabla_c\Phi^j)\nabla_d H \\ &= (\omega^{ad} - \mu_{bc}g^{ab}\omega^{cd})\nabla_d H,\end{aligned} \tag{25}$$

where we have defined

$$\mu_{bc} = M_{ij}\nabla_b\Phi^i\nabla_c\Phi^j. \tag{26}$$

It follows that we need to find whether the expression

$$\tilde{\omega}^{ab} = \omega^{ab} - g^{ad}\omega^{cb}\mu_{dc} \tag{27}$$

defines a symplectic structure on the subspace of the state space. Since the symplectic structure ω^{ab} is antisymmetric, we shall examine under which condition $\tilde{\omega}^{ab}$ is antisymmetric. This is equivalent to asking whether the following relation holds:

$$g^{ac}\omega^{bd}\mu_{cd} \overset{?}{=} -g^{bc}\omega^{ad}\mu_{cd}. \tag{28}$$

Suppose that (28) is valid. Then using (5) and (11) we can rewrite (28) as

$$g^{ac}g^{be}J_e^d\mu_{cd} = -g^{bc}g^{ae}J_e^d\mu_{cd}. \tag{29}$$

Transvecting this with g_{fa} and relabelling the indices we obtain

$$g^{be}J_e^d\mu_{ad} = -g^{bc}J_a^d\mu_{cd}, \tag{30}$$

from which it follows that

$$J_b^d\mu_{ad} = -J_a^d\mu_{bd}. \tag{31}$$

Multiplying both sides of (31) with J_c^a we find that condition (28) is equivalent to

$$J_a^cJ_b^d\mu_{cd} = \mu_{ab}, \tag{32}$$

where we have used (1) and the symmetry of μ_{ab}. It follows that for the metric formulation of the constrained motion (20) to be expressible in the Hamiltonian form (24) with the original Hamiltonian H, the matrix μ_{bc} defined by (26) must be Hermitian. This is the sufficiency condition that we set out to establish. Let us now examine specific cases to gain insight into this condition.

The case of a single constraint. In general, the J-invariance condition (32) need not be satisfied. One can easily see this by considering the case for which there is only one constraint given by $\Phi(x) = 0$. Then expression (18) becomes a scalar quantity, which we will denote by M, and thus its inverse is M^{-1}. It follows that

$$\mu_{ab} = M^{-1}\nabla_a\Phi\nabla_b\Phi. \tag{33}$$

Substituting this expression for μ_{ab} into (32) gives us

$$J_a^c\nabla_c\Phi J_b^d\nabla_d\Phi = \nabla_a\Phi\nabla_b\Phi, \tag{34}$$

which implies that

$$J_a^c\nabla_c\Phi = \nabla_a\Phi, \tag{35}$$

but this clearly is a contradiction, since the two vectors $J_a^c\nabla_c\Phi$ and $\nabla_a\Phi$ are *orthogonal*. We see therefore that in the case of a single constraint, condition (32) is not satisfied, and the constrained motion (20) cannot be expressed in the Hamiltonian form (24).

The case of two constraints. Let us examine the case in which there are two constraints. As we shall demonstrate, in this case the J-invariance condition for μ_{bc} reduces to a simpler condition. Let us write $\Phi^1 = A$ and $\Phi^2 = B$ for the two constraints. Then the inverse of the matrix M^{ij} can be written in the form

$$M_{ij} = \frac{1}{2\Delta}\epsilon_{ii'}\epsilon_{jj'}M^{i'j'}, \tag{36}$$

where $\Delta = \det(M^{ij})$, and ϵ_{ij} is a totally skew tensor with $i, i', j, j' = 1, 2$. Substituting (36) into (26) we find

$$\begin{aligned}
\mu_{bc} &= M_{ij}\nabla_b\Phi^i\nabla_c\Phi^j \\
&= \frac{1}{2\Delta}\epsilon_{ii'}\epsilon_{jj'}g^{pq}\nabla_p\Phi^{i'}\nabla_q\Phi^{j'}\nabla_b\Phi^i\nabla_c\Phi^j \\
&= \frac{1}{2\Delta}\epsilon_{ii'}\nabla_b\Phi^i\nabla_p\Phi^{i'}\epsilon_{jj'}\nabla_c\Phi^j\nabla_q\Phi^{j'}g^{pq} \\
&= \frac{1}{2\Delta}\tau_{bp}\tau_{cq}g^{pq},
\end{aligned} \tag{37}$$

where we have defined

$$\tau_{ab} = \epsilon_{ij}\nabla_a\Phi^i\nabla_b\Phi^j. \tag{38}$$

In order for (37) to satisfy (32) we thus require that

$$J_a^b\tau_{bc} = \pm\tau_{ab}J_c^b, \tag{39}$$

where we have substituted (37) into condition (32) and used $J_p^b J_q^c g^{pq} = g^{bc}$. Since

$$\tau_{ab} = \nabla_a A\nabla_b B - \nabla_a B\nabla_b A, \tag{40}$$

we find that (39) can be written more explicitly in the form

$$J_a^b\nabla_b A\nabla_c B - J_a^b\nabla_b B\nabla_c A = \pm\left(\nabla_a A J_c^b\nabla_b B - \nabla_a B J_c^b\nabla_b A\right). \tag{41}$$

Hence if this condition is satisfied (with either a plus or a minus sign) by the two constraints A and B, then the constrained equations of motion (20) take the form (24).

Holomorphic constraints. If we choose the constraint function to be holomorphic so that the two constraints A and B are given by the real and imaginary parts of

$$\Phi(x) = A(x) + \mathrm{i}B(x), \tag{42}$$

then we can find the form of τ_{ab} for which (39) holds. To obtain an expression for τ_{ab}, we recall that a real vector on Γ can be decomposed into its complex 'positive' and 'negative' parts $V_a = (V_\alpha, V_{\alpha'})$ (cf [13]). These components are given respectively by

$$(V_\alpha, 0) = \tfrac{1}{2}\left(V_a - \mathrm{i}J_a^b V_b\right) \qquad \text{and} \qquad (0, V_{\alpha'}) = \tfrac{1}{2}\left(V_a + \mathrm{i}J_a^b V_b\right). \tag{43}$$

Hence, $V_{\alpha'}$ is the complex conjugate of V_α, and these components are the eigenvectors of the complex structure J_b^a with eigenvalues $\pm\mathrm{i}$. It follows that if the vector is of type $V_a = (V_\alpha, 0)$ then $J_b^a V_a = \mathrm{i}V_b$, and similarly if $V_a = (0, V_{\alpha'})$ then $J_b^a V_a = -\mathrm{i}V_b$. With respect to this decomposition, the tensor τ_{ab} can be expressed as

$$\tau_{ab} = \begin{pmatrix} \tau_{\alpha\beta} & \tau_{\alpha\beta'} \\ \tau_{\alpha'\beta} & \tau_{\alpha'\beta'} \end{pmatrix}. \tag{44}$$

We rewrite condition (39) in the form

$$J_a^c J_b^d\tau_{cd} = \pm\tau_{ab} \tag{45}$$

by contracting both sides with J_d^c and using (1). In terms of decomposition (44) we find that in order for (45) to be true we require that τ_{ab} takes either of the two forms:

$$\tau_{ab}^{(+)} = \begin{pmatrix} 0 & \tau_{\alpha\beta'} \\ \tau_{\alpha'\beta} & 0 \end{pmatrix} \qquad \text{or} \qquad \tau_{ab}^{(-)} = \begin{pmatrix} \tau_{\alpha\beta} & 0 \\ 0 & \tau_{\alpha'\beta'} \end{pmatrix}, \tag{46}$$

where the plus and minus in $\tau_{ab}^{(\pm)}$ correspond to the required sign in (45). In view of (42) we can write the two constraints as $A(x) = \frac{1}{2}(\Phi + \bar{\Phi})$ and $B(x) = -\frac{1}{2}\mathrm{i}(\Phi - \bar{\Phi})$, where $\bar{\Phi}$ denotes the complex conjugate of Φ. Then we have

$$\begin{aligned} \nabla_\alpha A &= \tfrac{1}{2}\nabla_\alpha\Phi, & \nabla_\alpha B &= -\tfrac{1}{2}\mathrm{i}\nabla_\alpha\Phi, \\ \nabla_{\alpha'} A &= \tfrac{1}{2}\nabla_{\alpha'}\bar{\Phi}, & \nabla_{\alpha'} B &= \tfrac{1}{2}\mathrm{i}\nabla_{\alpha'}\bar{\Phi}. \end{aligned} \tag{47}$$

Using these expressions together with (40) we find that the components of $\tau_{ab}^{(-)}$ all vanish. Hence, when the two constraints A and B are given by (42), condition (39) is satisfied when τ_{ab} takes the form

$$\tau_{ab} = \begin{pmatrix} 0 & \tfrac{1}{2}\mathrm{i}\nabla_\alpha\Phi\nabla_{\beta'}\bar{\Phi} \\ -\tfrac{1}{2}\mathrm{i}\nabla_{\alpha'}\bar{\Phi}\nabla_\beta\Phi & 0 \end{pmatrix}, \tag{48}$$

i.e. when $\tau_{ab} = \tau_{ab}^{(+)}$. It follows that the metric formalism associated with holomorphic constraints of the form (42) is equivalent to the symplectic formalism.

We remark in general that the quadratic form $\tilde{\omega}^{ab}$ acting from the right annihilates the vector $\nabla_a\Phi^k$ normal to the constraint surface. This can be verified explicitly as follows:

$$\begin{aligned}\tilde{\omega}^{ad}\nabla_a\Phi^k &= \omega^{ad}\nabla_a\Phi^k - M_{ij}g^{ab}\nabla_b\Phi^i\nabla_a\Phi^k\omega^{cd}\nabla_c\Phi^j\\ &= \omega^{ad}\nabla_a\Phi^k - M_{ij}M^{ki}\omega^{cd}\nabla_c\Phi^j\\ &= \omega^{ad}\nabla_a\Phi^k - \omega^{ad}\nabla_a\Phi^k\\ &= 0, \end{aligned}\tag{49}$$

since $g^{ab}\nabla_a\Phi^k\nabla_b\Phi^i = M^{ki}$ and $M_{ij}M^{ki} = \delta^k_j$. This condition, of course, is equivalent to the condition that $\dot{x}^a\nabla_a\Phi^k = 0$. However, in general we have

$$\tilde{\omega}^{ad}\nabla_d\Phi^k \neq 0,\tag{50}$$

since $\tilde{\omega}^{ab}$ is not necessarily antisymmetric. In other words, the vanishing of the left-hand side of (50) is equivalent to the J-invariance condition for μ_{bc}.

In summary, the procedure for deriving the equations of motion in the metric approach to constrained quantum motion is as follows. First, express the relevant constraints in the form $\{\Phi^i(x) = 0\}_{i=1,2,\ldots,N}$. Determine the matrix M^{ij} via (18). Assuming that M^{ij} is nonsingular, calculate its inverse M_{ij}. Substitute the result into (20) and we recover the relevant equations of motion. Having obtained the general procedure, let us now examine some explicit examples implementing this procedure.

5. Illustrative examples

Example 1. The first example that we consider here is identical to the one considered in [4] involving a pair of spin-$\frac{1}{2}$ particles. We consider the subspace of the state space associated with product states upon which all the energy eigenstates lie. An initial state that lies on this product space is required to remain a product state under the evolution generated by a generic Hamiltonian. In this example there are two constraints $\Phi^1(x)$ and $\Phi^2(x)$, and we shall show that the metric approach introduced here gives rise to a result that agrees with the one obtained in [4] using the symplectic approach.

Let us work with the coordinates of the quantum state space given by the 'action-angle' variables [4, 14], where the canonical conjugate variables are given by $\{x^a\} = \{q_\nu, p_\nu\}_{\nu=1,\ldots,n-1}$ such that when generic pure states $|x\rangle$ are expanded in terms of the energy eigenstates $\{|E_\alpha\rangle\}_{\alpha=1,\ldots,n}$, the associated amplitudes are given by $\{p_\nu\}$ and the relative phases by $\{q_\nu\}$. In the case of a pair of spin-$\frac{1}{2}$ particles we can thus expand a generic state in the form

$$|x\rangle = \sqrt{p_1}\,\mathrm{e}^{-\mathrm{i}q_1}|E_1\rangle + \sqrt{p_2}\,\mathrm{e}^{-\mathrm{i}q_2}|E_2\rangle + \sqrt{p_3}\,\mathrm{e}^{-\mathrm{i}q_3}|E_3\rangle + \sqrt{1-p_1-p_2-p_3}|E_4\rangle.\tag{51}$$

This choice of coordinates has the property that if we write

$$H(p,q) = \frac{\langle x|H|x\rangle}{\langle x|x\rangle}\tag{52}$$

for the Hamiltonian, where $|x\rangle = |p,q\rangle$, then the Schrödinger equation is expressed in the form of the conventional Hamilton equations:

$$\dot{q}_\nu = \frac{\partial H(q,p)}{\partial p_\nu} \qquad \text{and} \qquad \dot{p}_\nu = -\frac{\partial H(q,p)}{\partial q_\nu}.\tag{53}$$

In the energy basis the Hamiltonian can be expressed as

$$H = \sum_{\alpha=1}^{4} E_\alpha|E_\alpha\rangle\langle E_\alpha|.\tag{54}$$

It follows that the phase space function $H(p,q)$ for a generic Hamiltonian is given by

$$H = E_4 + \sum_{\nu=1}^{3} \omega_\nu p_\nu, \tag{55}$$

where $\omega_\nu = E_\nu - E_4$. The symplectic structure and its inverse in these coordinate (recall the relation $\omega^{ac}\omega_{bc} = \delta^a_b$) are thus given respectively by

$$\omega_{ab} = \begin{pmatrix} \mathbb{O} & \mathbb{1} \\ -\mathbb{1} & \mathbb{O} \end{pmatrix} \qquad \text{and} \qquad \omega^{ab} = \begin{pmatrix} \mathbb{O} & \mathbb{1} \\ -\mathbb{1} & \mathbb{O} \end{pmatrix}, \tag{56}$$

where $\mathbb{1}$ is the 2×2 identity matrix and $\mathbb{O}$ is the 2×2 null matrix.

Let us write $\{\psi^\alpha\}_{\alpha=1,2,3,4}$ for the coefficients of the energy eigenstates in (51). Then the constraint equation is expressed in the form $\psi^1\psi^4 = \psi^2\psi^3$, which is just a single complex equation [4]. Thus in real terms we have two constraints given by

$$\begin{cases} \Phi^1 = \sqrt{p_1p_4}\cos q_1 - \sqrt{p_2p_3}\cos(q_2+q_3) = 0, \\ \Phi^2 = \sqrt{p_1p_4}\sin q_1 - \sqrt{p_2p_3}\sin(q_2+q_3) = 0. \end{cases} \tag{57}$$

These constraints are 'separable' and can be rewritten as

$$\begin{cases} \Phi^1 = q_1 - q_2 - q_3 = 0, \\ \Phi^2 = p_1(1-p_1-p_2-p_3) - p_2p_3 = 0. \end{cases} \tag{58}$$

The next step in the metric approach for the constraint is to work out the expression for the Fubini–Study metric associated with the line element:

$$\mathrm{d}s^2 = 8\left[\frac{\psi^{[\alpha}\,\mathrm{d}\psi^{\beta]}\bar{\psi}_{[\alpha}\,\mathrm{d}\bar{\psi}_{\beta]}}{(\bar{\psi}_\gamma\psi^\gamma)^2}\right] \tag{59}$$

in terms of the canonical variables $\{q_\nu, p_\nu\}_{\nu=1,2,3}$. A calculation shows that

$$g_{ab} = \begin{pmatrix} 4(1-p_1)p_1 & -4p_1p_2 & -4p_1p_3 & 0 & 0 & 0 \\ -4p_1p_2 & 4(1-p_2)p_2 & -4p_2p_3 & 0 & 0 & 0 \\ -4p_1p_3 & -4p_2p_3 & 4(1-p_3)p_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-p_2-p_3}{p_1p_4} & \frac{1}{p_4} & \frac{1}{p_4} \\ 0 & 0 & 0 & \frac{1}{p_4} & \frac{1-p_1-p_3}{p_2p_4} & \frac{1}{p_4} \\ 0 & 0 & 0 & \frac{1}{p_4} & \frac{1}{p_4} & \frac{1-p_1-p_2}{p_3p_4} \end{pmatrix}, \tag{60}$$

where for simplicity we have denoted $p_4 = 1 - p_1 - p_2 - p_3$. The inverse is thus:

$$g^{ab} = \begin{pmatrix} \frac{1-p_2-p_3}{4p_1p_4} & \frac{1}{4p_4} & \frac{1}{4p_4} & 0 & 0 & 0 \\ \frac{1}{4p_4} & \frac{1-p_1-p_3}{4p_2p_4} & \frac{1}{4p_4} & 0 & 0 & 0 \\ \frac{1}{4p_4} & \frac{1}{4p_4} & \frac{1-p_1-p_2}{4p_3p_4} & 0 & 0 & 0 \\ 0 & 0 & 0 & (1-p_1)p_1 & -p_1p_2 & -p_1p_3 \\ 0 & 0 & 0 & -p_1p_2 & (1-p_2)p_2 & -p_2p_3 \\ 0 & 0 & 0 & -p_1p_3 & -p_2p_3 & (1-p_3)p_3 \end{pmatrix}. \tag{61}$$

To obtain explicit expressions for equations of motion (20) we need to calculate the matrix M^{ij} and its inverse. A short calculation shows that

$$M^{ij} = \begin{pmatrix} \frac{1}{4}\left(\frac{1}{p_1}+\frac{1}{p_2}+\frac{1}{p_3}+\frac{1}{p_4}\right) & 0 \\ 0 & \begin{matrix} p_1p_4(1-4p_1p_4+4p_2p_3) \\ +(p_2+p_3-4p_2p_3)(p_2p_3-p_1p_4) \end{matrix} \end{pmatrix}, \tag{62}$$

from which its inverse M_{ij} can easily be obtained. Putting these together, we find that the equations of motion are given by

$$\begin{aligned}
\dot{q}_1 &= \omega_1 - \frac{p_2 p_3(1-2p_1-p_2-p_3)(\omega_1-\omega_2-\omega_3)}{p_2p_3(1-p_2-p_3)-p_1^2(p_2+p_3)+p_1(1-p_2-p_3)(p_2+p_3)},\\
\dot{q}_2 &= \omega_2 + \frac{p_1 p_3(1-p_1-p_3)(\omega_1-\omega_2-\omega_3)}{p_2p_3(1-p_2-p_3)-p_1^2(p_2+p_3)+p_1(1-p_2-p_3)(p_2+p_3)},\\
\dot{q}_3 &= \omega_3 + \frac{p_1 p_2(1-p_1-p_2)(\omega_1-\omega_2-\omega_3)}{p_2p_3(1-p_2-p_3)-p_1^2(p_2+p_3)+p_1(1-p_2-p_3)(p_2+p_3)},\\
\dot{p}_1 &= 0,\\
\dot{p}_2 &= 0,\\
\dot{p}_3 &= 0.
\end{aligned} \tag{63}$$

We can simplify the equations using the relation $p_1p_4 = p_2p_3$, which gives us

$$\begin{aligned}
\dot{q}_1 &= \omega_1 - (1-2p_1-p_2-p_3)(\omega_1-\omega_2-\omega_3),\\
\dot{q}_2 &= \omega_2 + (p_1+p_3)(\omega_1-\omega_2-\omega_3),\\
\dot{q}_3 &= \omega_3 + (p_1+p_2)(\omega_1-\omega_2-\omega_3),\\
\dot{p}_1 &= 0,\\
\dot{p}_2 &= 0,\\
\dot{p}_3 &= 0.
\end{aligned} \tag{64}$$

These equations are precisely those obtained in [4] by means of the symplectic formalism. The solutions to these equations are also worked out in [4].

Before we proceed to the next example, let us verify explicitly that condition (32) for the equivalence of the metric and symplectic approaches indeed holds in this example. For this we need to obtain the expression for the complex structure in the canonical coordinates $\{q_\nu, p_\nu\}_{\nu=1,2,3}$ using relations (5) and (11). This is given by

$$J^a_b = \begin{pmatrix}
0 & 0 & 0 & \frac{1-p_2-p_3}{2p_1p_4} & \frac{1}{2p_4} & \frac{1}{2p_4}\\
0 & 0 & 0 & \frac{1}{2p_4} & \frac{1-p_1-p_3}{2p_2p_4} & \frac{1}{2p_4}\\
0 & 0 & 0 & \frac{1}{2p_4} & \frac{1}{2p_4} & \frac{1-p_1-p_2}{2p_3p_4}\\
2(p_1-1)p_1 & 2p_1p_2 & 2p_1p_3 & 0 & 0 & 0\\
2p_1p_2 & 2(p_2-1)p_2 & 2p_2p_3 & 0 & 0 & 0\\
2p_1p_3 & 2p_2p_3 & 2(p_3-1)p_3 & 0 & 0 & 0
\end{pmatrix}, \tag{65}$$

where as before we write $p_4 = 1 - p_1 - p_2 - p_3$. Substituting this expression and the expression for μ_{ab} obtained from (26) into (32), we find that the condition is indeed satisfied.

Example 2. Consider a single spin-$\frac{1}{2}$ particle system immersed in a z-field with a unit strength. The space of pure states for this system is just the surface of the Bloch sphere. The Hamiltonian of the system is given by $\hat{H} = \hat{\sigma}_z$, where $\hat{\sigma}_z$ is the Pauli spin matrix in the z-direction. We then impose the constraint that an observable, say $\hat{\sigma}_x$, that does not commute with the Hamiltonian, must be conserved under the time evolution.

As before we chose the canonical coordinates $x^a = \{q, p\}$ for the Bloch sphere by setting

$$|x(p,q)\rangle = \sqrt{1-p}|E_1\rangle + \sqrt{p}\,\mathrm{e}^{-\mathrm{i}q}|E_2\rangle. \tag{66}$$

The Hamiltonian in this coordinate system is given by

$$H(q,p) = 1 - 2p. \tag{67}$$

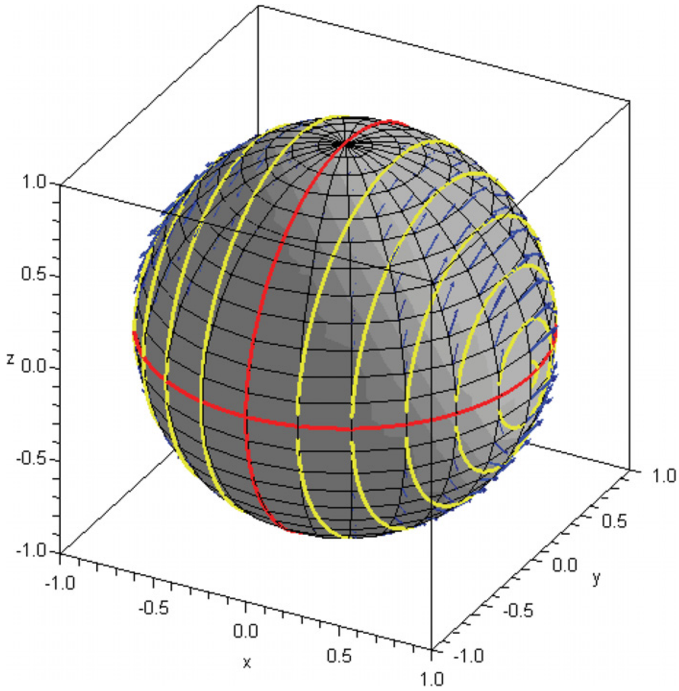

Figure 1. A field plot of the dynamics resulting from a system constrained to remain on a surface defined by $\Phi = \hat{\sigma}_x$ when the system evolves according to the Hamiltonian $H = \hat{\sigma}_z$, where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are Pauli matrices. Shown in yellow/light grey lines are the integral curves of the motion resulting when we choose as the starting positions $\{\theta_1, \phi_n\} = \{\frac{23\pi}{48}, \frac{2\pi n}{24}\}_{n=0,\ldots,23}$ and $\{\theta_2, \phi_n\} = \{\frac{25\pi}{48}, \frac{2\pi n}{24}\}_{n=0,\ldots,23}$. The great circles shown in red/thick grey lines, the equators of the x and z-axes, consist of fixed points. A state that initially lies on one of these great circles does not move away from that point, whereas all other states evolve asymptotically towards the fixed point where the associated integral curve intersects the equator of the sphere.

(This figure is in colour only in the electronic version)

The conservation of $\hat{\sigma}_x$ then reduces to a single real constraint of the form $\langle x|\hat{\sigma}_x|x\rangle = \text{constant}$, which, by use of (66), gives us

$$\Phi(x) = 2\sqrt{p(1-p)}\cos q. \tag{68}$$

The metric on the Bloch sphere, in terms of our conjugate variables, is given by

$$g_{ab} = \begin{pmatrix} 4(1-p)p & 0 \\ 0 & \frac{1}{(1-p)p} \end{pmatrix}. \tag{69}$$

The symplectic structure has the same form as (56) so we can now calculate the scalar quantity M defined in (18). A short calculation shows that

$$M = (1-2p)^2\cos^2 q + \sin^2 q. \tag{70}$$

Evidently M vanishes at a pair of points $(p, q) = (1/2, 0)$ and $(p, q) = (1/2, \pi)$ of Γ, i.e. the fixed points of the constrained observable $\hat{\sigma}_x$. These are also the fixed points of the constrained motion. Thus assuming $M \neq 0$ and substituting (70) into (20) we find that the equations of motion are given by

$$\dot{q} = \frac{-2(1-2p)^2\cos^2 q}{(1-2p)^2\cos^2 q + \sin^2 q} \tag{71}$$

and

$$\dot{p} = \frac{4(1-2p)(-1+p)p\sin q\cos q}{(1-2p)^2\cos^2 q + \sin^2 q}. \tag{72}$$

In order to visualize the results we convert the equations of motion into angular coordinates, using the method outlined in [4]. In angular coordinates (66) is given by

$$|x(\theta,\phi)\rangle = \cos\tfrac{1}{2}\theta|E_1\rangle + \sin\tfrac{1}{2}\theta\,\mathrm{e}^{\mathrm{i}\phi}|E_2\rangle. \tag{73}$$

Comparing (66) and (73) we make the identification $p = \sin^2\frac{1}{2}\theta$ and $q = -\phi$. The equations of motion then become

$$\dot{\theta} = \frac{1}{2}\left(\frac{\sin(2\theta)\sin(2\phi)}{1-\sin^2\theta\cos^2\phi}\right) \qquad \text{and} \qquad \dot{\phi} = \frac{2\cos^2\theta\cos^2\phi}{1-\sin^2\theta\cos^2\phi}. \tag{74}$$

Figure 1 shows some of the integral curves resulting from the above equations, plotted on the surface of the Bloch sphere. Equation (74) is valid at all points except where $(\theta,\phi) = \left(\frac{\pi}{2},0\right)$ and $(\theta,\phi) = \left(\frac{\pi}{2},\pi\right)$ corresponding to the two fixed points of $\hat{\sigma}_x$ mentioned above.

It is also straightforward to verify that the results above could not have been obtained using the symplectic approach. The complex structure on the underlying state space of the spin-$\frac{1}{2}$ particle in our coordinate system is given by

$$J^a_b = \begin{pmatrix} 0 & \frac{1}{2(1-p)p} \\ -2(1-p)p & 0 \end{pmatrix}. \tag{75}$$

Evaluating (26) using (70), and substituting the result along with (75) into (32), we find that (32) does not hold.

References

[1] Burić N 2007 Hamiltonian quantum dynamics with separability constraints *Ann. Phys.* **323** 17–33

[2] Corichi A 2008 On the geometry of quantum constrained systems *Class. Quantum Grav.* **25** 135013

[3] Graefe E M, Korsch H J and Niederle A E 2008 Mean-field dynamics of a non-Hermitian Bose–Hubbard dimer *Phys. Rev. Lett.* **101** 150408

[4] Brody D C, Gustavsson T A C and Hughston L P 2008 Symplectic approach to quantum constraints *J. Phys. A: Math. Theor.* **41** 475301

[5] Dirac M P A 1950 Generalized Hamiltonian dynamics *Can. J. Math.* **2** 129–48

[6] Dirac M P A 1958 Generalised Hamiltonian dynamics *Proc. R. Soc. Lond.* A **246** 326–32

[7] Kibble B T W 1979 Geometrisation of quantum mechanics *Commun. Math. Phys.* **65** 189–201

[8] Cirelli R, Mania A and Pizzocchero L 1990 Quantum mechanics as an infinite-dimensional Hamiltonian system with uncertainty structure: I, II *J. Math. Phys.* **31** 2891–903

[9] Hughston L P 1995 Geometric aspects of quantum mechanics *Twistor Theory* ed S Huggett (New York: Dekker)

[10] Ashtekar A and Schilling T A 1995 Geometry of quantum mechanics *CAM-94 Physics Meeting* (*AIP Conf. Proc.* vol 342) ed A Zapeda (Woodbury, New York: AIP Press) pp 471–8

[11] Brody D C and Hughston L P 2001 Geometric quantum mechanics *J. Geom. Phys.* **38** 19–53

[12] Newlander A and Nirenberg L 1957 Complex analytic coordinates in almost complex manifolds *Ann. Math.* **65** 391–404

[13] Brody D C and Hughston L P 1998 Statistical geometry in quantum mechanics *Proc. R. Soc. Lond.* A **454** 2445–75

[14] Oh P and Kim M 1994 Action angle variables for complex projective space and semiclassical exactness *Mod. Phys. Lett.* A **9** 3339–46