Constrained quantum dynamics

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Abstract. We give an overview of the two different methods that have been introduced in order to describe the dynamics of constrained quantum systems; the symplectic formulation and the metric formulation. The symplectic method extends the work of Dirac on constrained classical systems to quantum systems, whereas the metric approach is purely a quantum mechanical method having no immediate classical counterpart. Two examples are provided that illustrate the nonlinear motion induced by the constraint.

1. Introduction
A question that has recently been asked is how does one implement unitary motion on a quantum system that is subject to a set of constraints? In classical mechanics, constrained evolutions are often constructed using an approach developed by Dirac [1, 2], which uses the symplectic geometry of the classical phase space. Recently, several authors [3, 4, 5] have worked on extending the classical theory of constraint to quantum systems, using the phase space formulation of quantum mechanics. There are, however, pros and cons in this approach: It is for example only applicable to systems subject to an even number of constraints. To address this and other issues, an alternative approach for treating constrained quantum systems was introduced in [6]. In this paper we review both these approaches and explore through examples the kind of nonlinear motion that results from constraining a unitary evolution in quantum mechanics.

The classical method uses the property that the classical phase space is a symplectic manifold endowed with a symplectic structure. The quantum mechanical phase space has the geometry of a Kähler manifold, with both a symplectic structure and a metric structure. As the method considered by [3, 4, 5] uses the symplectic geometry of the quantum phase space, it was given the name the symplectic approach to quantum constraints [5]. The alternative formalism introduced in [6] makes a novel use of the metric structure of the quantum state space, thus referred to as the metric approach to quantum constraints.

In this paper we will first review some of the main features of the phase space formulation of quantum mechanics. We will then highlight the key features of both the symplectic and metric approaches to implementing constrained unitary motion and discuss the resulting evolutions by looking at two examples.

2. The phase-space formulation of quantum mechanics
The phase space description of quantum mechanics is based on a projective Hilbert space formulation (see for example [7, 8, 9, 10, 11, 12, 13, 14, 15] and references cited therein). The idea is as follows. The expectation value of any observable in quantum mechanics is independent
of the norm of the state vector

$$|x\rangle \sim \lambda|x\rangle \quad \lambda \in \mathbb{C} - \{0\}. \quad (1)$$

A state in quantum mechanics can hence be viewed as a ray through the origin of the Hilbert space $\mathcal{H}^{n+1}$, and we can, without loss of any physical information about the system, consider quantum mechanics in the space of rays. The space of rays correspond to the complex projective space $\mathbb{P}^n$, where each state of the system is now given by a point. In real terms $\mathbb{P}^n$ is an even dimensional manifold $\Gamma_{2n}$ equipped with a Riemannian structure given by the Fubini-Study metric $g_{\alpha \beta}$ and a compatible symplectic structure $\Omega_{\alpha \beta}$. The transition probability between two states in $\Gamma$ is given by the associated geodesic distance between the two points. It is interesting to note that the probabilistic aspects of quantum theory are hence associated with the underlying metric geometry of the state space. In comparison the dynamical aspects of the theory are captured by underlying symplectic geometry. Physical observables are functions on $\Gamma$ given by the expectation value of the corresponding Hilbert space operator at each point $x$. The Hamiltonian, for example, is given by

$$H(x) = \frac{\langle x|H|x\rangle}{\langle x|x\rangle}. \quad (2)$$

The eigenstates of the Hamiltonian are given by the fixed points of $H$:

$$\nabla_a H(x) = 0, \quad (3)$$

and the corresponding eigenvalues are the values of $H(x)$ at each fixed point. Unitary evolution is governed by the Schrödinger equation, which takes the form of Hamilton’s equations:

$$\frac{dx^a}{dt} = \Omega^{ab} \nabla_b H(x), \quad (4)$$

where $\Omega^{ab}$ is the inverse symplectic structure given by $\Omega_{ab}\Omega^{bc} = -\delta^c_a$. Here, and throughout the paper, there is an implied summation over repeated indices. We parameterise the state space by the “action-angle” parameterisation (cf. [16]) so that the equations of motion (4) take a particularly simple and familiar form. If we let the state $|x\rangle$ in energy basis be given by

$$|x\rangle = \sum_{i=1}^n \sqrt{p_i} e^{-ip_i} |E_i\rangle + \sqrt{1 - \sum_{i=1}^n p_i |E_{n+1}\rangle}, \quad (5)$$

then the expectation of the Hamiltonian operator $\hat{H} = \sum_j E_j |E_j\rangle \langle E_j|$ is given by

$$H(q_i, p_i) = E_{n+1} + \sum_{i=1}^n \omega_i p_i, \quad \text{where} \quad \omega_i = E_i - E_{n+1}. \quad (6)$$

The equations of motion then take the form

$$\dot{q}_i = \frac{\partial H(q_i, p_i)}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H(q_i, p_i)}{\partial q_i}, \quad (7)$$

with solutions $q_i(t) = q_i(0) + \omega_i t$ and $p_i(t) = p_i(0)$. 


3. Constrained dynamics

Let us now assume that the evolution of the quantum system is subject to one or more constraints. The type of constraints that we will be considering can be written in the form

$$\Phi^i(x) = 0, \quad i = 1, 2, \ldots, N,$$

(8)

where $N$ is the total number of constraints. Equation (8) defines a subspace $\Phi$ of $\Gamma$, given by the intersection of each of the $N$ subspaces defined by $\Phi^i = 0$, onto which the evolution will be constrained, see figure 1.

We shall here consider two different types of constraints. The first type is given by the conservation of a set of observables, i.e.

$$\Phi^i(x) = \frac{\langle x|\hat{\Phi}^i|x \rangle}{\langle x|x \rangle},$$

(9)

where $\hat{\Phi}^i$ is the Hilbert space operator corresponding to the observable $\Phi^i$. The second type of constraint is when the evolution of the system is constrained to an algebraically well defined subspace of $\Gamma$ that does not correspond to the conservation of any observable. An example of this is to constrain the motion of a pair of spin-$\frac{1}{2}$ particles that are initially disentangled to remain disentangled. There is no observable that corresponds to this property of the system, but as disentangled states form a subspace $Q = \mathbb{P}^1 \times \mathbb{P}^1$ [15, 17] of the overall state space $\mathbb{P}^3$ (see figure 2), we can constrain the system algebraically to remain on this subspace. We shall return to this example and look at it in more detail in the next section where we give an outline of the symplectic approach to implementing quantum constraints.

Figure 1. The constraints $\Phi^i = 0$ define a subspace of $\Gamma$. The evolution of the system can be constrained to this subspace using either the symplectic or the metric method. When using the symplectic approach the modified equations of motion take the same form as the original one, but with a modified symplectic structure $\tilde{\Omega}_{ab}$. In the metric approach the system is constrained by removing all components orthogonal to the surface from the vector field $\dot{x}^a = \Omega^{ab}\nabla_b H$.

Figure 2. The state space of 2 spin-$\frac{1}{2}$ particles. The disentangled states form a subspace of the total state space given by $Q = \mathbb{P}^1 \times \mathbb{P}^1$, where $\mathbb{P}^1$ is the complex projective line. Further details of the state space structure of this system can be found in [15, 17].
3.1. Symplectic approach
Let us first consider the symplectic approach and follow the methodology introduced in [5]. In order to implement the constraints (8) the equations of motion are modified such that

$$\frac{dx^a}{dt} = \Omega^{ab} \nabla_b H(x) + \lambda_i \Omega^{ab} \nabla_b \Phi_i(x), \tag{10}$$

where $\lambda_i$ are Lagrange multipliers associated with the constraints $\Phi_i(x)$. In some cases these Lagrange multipliers can be found explicitly by considering $\dot{\Phi}_i = 0$. By expanding $\dot{\Phi}_i$ using the chain rule $\dot{\Phi}_i = \dot{x}^a \nabla_a \Phi_i$ we find that the Lagrange multiplier is given by:

$$\lambda_i = \omega_{ji} \Omega^{ab} \nabla_a \Phi_j \nabla_b H, \tag{11}$$

where $\omega_{ij}$, assuming it exists, is the inverse of $\omega_{ij} := \Omega^{ab} \nabla_a \Phi_i \nabla_b \Phi_j$.

(12)

Note that when the constraints are given by conserved observables (9), then $\omega^{ij}$ correspond to the commutator between the two observables. By substituting the Lagrange multipliers back into (10) we find that the equations of motion can be rewritten in the form [5]

$$\frac{dx^a}{dt} = \tilde{\Omega}^{ab} \nabla_b H(x), \tag{13}$$

where $\tilde{\Omega}^{ab}$ is the induced symplectic structure on the constraint subspace $\Phi^i = 0$ given by

$$\tilde{\Omega}^{ab} = \Omega^{ab} + \Omega^{ac} \Omega^{bd} \omega_{ij} \nabla_c \Phi_i \nabla_d \Phi_j. \tag{14}$$

In other words, the equations of motion for the constrained system take the same form as for the unconstrained system. Only the symplectic structure is no longer the globally defined $\Omega_{ab}$, but the symplectic structure induced locally on the subspace $\Phi^i = 0$ (see figure 1). A consequence of this is that we can no longer expect the resulting motion to be unitary, as the induced symplectic structure $\tilde{\Omega}_{ab}$ has a nonlinear term. In order to illustrate the kind of motion that could result from this kind of constraint we consider the example of two spin-$\frac{1}{2}$ particles constrained to remain disentangled, as mentioned above. Let us first note however that the symplectic approach is not applicable to all systems. In order to use it, one requirement is that $N$, the total number of constraints being imposed, must be even. This follows by construction as otherwise the symplectic geometry is not preserved on the constraint surface. Another condition that must be satisfied in order to find the lagrange multipliers is that the inverse of (12) must exist.

Example 1: Let us now consider the example of two spin-$\frac{1}{2}$ particles with Hamiltonian:

$$\hat{H} = -J \hat{\sigma}_1 \otimes \hat{\sigma}_2 - B (\hat{\sigma}_z^1 \otimes 1_2 + 1_1 \otimes \hat{\sigma}_z^2), \tag{15}$$

where the subscripts 1 and 2 labels the two particles, $J$ is the strength of the spin-interaction, $B$ is the strength of the external magnetic field (orientated along the z-axis), and $\hat{\sigma}_z$ is the Pauli spin matrix in the z-direction. We further require the initial state to be disentangled, and we wish to constrain the system so that it remains so. In other words we want the state of the system to remain on the surface $Q = \mathbb{P}^1 \times \mathbb{P}^1$ as it evolves. To find the equations of motion we follow the method outlined above, first finding (12), taking its inverse, using it to evaluate the Lagrange multipliers and hence finding $\tilde{\Omega}_{ab}$ (please see [5] for full details of this calculation).

Since the complex projective line is isomorphic to the two-sphere $\mathbb{P}^1 \sim \mathbb{S}^2$, we can view $Q$ as the product space of a pair of 2-spheres $\mathbb{S}^2_1 \times \mathbb{S}^2_2$. Changing coordinates into spherical coordinates...
(see [5]) we can visualise the evolution on the surface of the 2-spheres. The resulting equations of motion consist of four coupled non-linear differential equations:

\[
\begin{align*}
\dot{\theta}_1 &= \sin(\phi_1 - \phi_2) \sin \theta_2 \left[(\omega_1 - \omega_2) \cos \theta_1 + \omega_2 - \omega_3\right] \\
\dot{\theta}_2 &= \sin(\phi_1 - \phi_2) \sin \theta_1 \left[(\omega_2 - \omega_1) \cos \theta_2 - \omega_2 + \omega_3\right] \\
\dot{\phi}_1 &= \frac{1}{2} \left[-\omega_1 + (\omega_2 - \frac{\omega_1}{2}) \cos \theta_1 + \frac{3}{2} \left(\omega_1 - \omega_2 - 2\omega_3\right) \cos \theta_1 + \cos(\phi_1 - \phi_2)/(\sin \theta_1 \sin \theta_2)\right] \\
& \quad \times \left(2(\omega_3 - \omega_2) \sin^2 \theta_1 \cos \theta_2 + (\omega_1 - \omega_2)(\cos^2 \theta_1 - \cos^2 \theta_2)\right) \\
\dot{\phi}_2 &= \frac{1}{2} \left[-\omega_1 + (\omega_2 - \frac{\omega_1}{2}) \cos \theta_1 + \frac{3}{2} \left(\omega_1 - \omega_2 - 2\omega_3\right) \cos \theta_2 + \cos(\phi_1 - \phi_2)/(\sin \theta_1 \sin \theta_2)\right] \\
& \quad \times \left(2(\omega_3 - \omega_2) \cos \theta_1 \sin^2 \theta_2 - (\omega_1 - \omega_2)(\cos^2 \theta_1 - \cos^2 \theta_2)\right)
\end{align*}
\] (16)

It is difficult to solve these equations of motion in closed form. We will therefore explore the solution numerically by looking at various ‘snapshots’ of the vector field and associated trajectories as the system passes through certain points. In figure 3 we see four examples of this. The top left picture shows us the vector field on \(S_1^2\) as the evolution on \(S_2^2\) passes through the point \(\theta_2 = \phi_2 = \frac{\pi}{2}\). As the overall state of the system changes, we evolve on both spheres and as we change state on \(S_1^2\) the vector field on \(S_2^2\) changes and vice versa. To fully explore the solution numerically, we require an ‘interactive simulation’; figure 3 merely gives a flavour for the often complicated trajectories that result from constraining the system to remain on \(Q\). The strength of the formalism is that the solutions are nonetheless fully tractable, at least numerically.

3.2. Metric approach

In the previous section we found that there is a way to implement quantum constraints using the underlying symplectic geometry of the phase space. Let us now look at how some of the
limitations of the symplectic formalism can be overcome by using the metric geometry of the phase space.

Another way of constraining the evolution of a system whose initial state lies on the surface \( \Phi = 0 \) is to remove all the components of the vector field normal to it [6] (see figure 1). This will force the system to remain on \( \Phi = 0 \). To implement this constraint we still use the method of Lagrange multipliers, but we substitute the symplectic structure in the second term of (10) with the metric structure. Hence the modified equations of motion become:

\[
\frac{dx^a}{dt} = \Omega^{ab} \nabla_b H - \lambda_i g^{ab} \nabla_b \Phi^i, \tag{17}
\]

where \( g^{ab} \) is the inverse of the Fubini-Study metric. Because we are now making use of the metric geometry of the constraint subspace, we no longer require that the total number of constraints \( N \) be even. The Lagrange multipliers \( \lambda_i \) can again be found explicitly in a similar way to the previous approach by considering \( \dot{\Phi}^i = 0 \). Following the method in [6], we hence find that

\[
\lambda_i = M_{ij} \Omega^{cd} \nabla_c \Phi^j \nabla_d H, \tag{18}
\]

where \( M_{ij} \) is the inverse of the matrix

\[
M^{ij} := g^{ab} \nabla_a \Phi^i \nabla_b \Phi^j. \tag{19}
\]

For the case when the constraints correspond to a family of conserved quantum observables, the matrix \( M^{ij} \) corresponds to the anticommutators between the observables. We hence require \( \det(M^{ij}) \neq 0 \) in order to find the equations of motion:

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

It is no longer in general the case that these can be rewritten in the form \( \dot{x}^a = \tilde{\Omega}^{ab} \nabla_b H \), where \( \tilde{\Omega}^{ab} \) is the inverse of a modified symplectic structure. We would, however, expect that systems that can be treated with both methods return the same result. It turns out that this is very hard to verify in general. In [6], a sufficient condition was derived under which the metric approach reduces to the symplectic approach with the modified equations of motion taking the form of (13), (see [6] for further details on this). We therefore take the view that the metric approach is the more general way of treating quantum constraints, but under certain conditions it reduces to an extension of the classical method to quantum systems as in the symplectic approach. We shall now look at one of the simplest examples of a system subject to only one constraint.

**Example 2:** Let us consider the example of a single spin-\( \frac{1}{2} \) particle with Hamiltonian \( \hat{H} = \hat{\sigma}_z \), where \( \hat{\sigma}_z \) is a Pauli spin matrix, constrained such that

\[
\Phi(x) = \frac{\langle x | \hat{\sigma}_z | x \rangle}{\langle x | x \rangle} \tag{21}
\]

is conserved [6]. This example is interesting as we have an observable that does not commute with the Hamiltonian. Following the method outlined above, the equations of motion are obtained by considering (19), taking its inverse, finding the Lagrange multipliers (18) and hence the equations of motion (20). Just as in the previous example we look at the problem in spherical coordinates to more easily visualise the resulting evolution as trajectories on the surface of the 2-sphere. The modified equations of motion are given by [6]

\[
\dot{\theta} = \frac{1}{2} \left( \frac{\sin(2\theta) \sin(2\phi)}{1 - \sin^2 \theta \cos^2 \phi} \right), \quad \text{and} \quad \dot{\phi} = \frac{2 \cos^2 \theta \cos^2 \phi}{1 - \sin^2 \theta \cos^2 \phi}. \tag{22}
\]
Figure 4. The vector field resulting from a single spin-$\frac{1}{2}$ particle with Hamiltonian $\hat{H} = \sigma_z$ being constrained such that $A(x) = \frac{\langle x|\sigma_z|x\rangle}{\langle x|x\rangle}$ is conserved [6]. The yellow lines are integral curves of the vector field and the red lines correspond to fixed points.

Figure 4 shows the resulting vector field and some of its integral curves. We recall that unitary unconstrained motion for this system corresponds to rigid rotation around the $z$-axis. As we are now forcing the system to remain on $\langle \sigma_x \rangle = 0$, corresponding to circles around the $x$-axis, the resulting solution has a very interesting fixed point structure. Instead of only having two fixed points, the poles along the $z$-axis, as in the unconstrained case, the state space is now effectively partitioned into quarters of the sphere that do not interact with each other. Systems whose initial state is not a fixed point hence evolve along the half circular trajectories towards the fixed points along the equator.

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