Quantizing conditionally variational nonholonomic systems

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Abstract

In this paper we present a quantization procedure for a class of nonholonomic systems—briefly, mechanical systems subject to nonintegrable constraints on the velocities—whose reduced mechanics is Hamiltonian. We illustrate the theory developed through several examples, one of which demonstrates how the classical nonholonomic constraints are sometimes manifested quantum mechanically as a shift in the ground state energy of the system.

Keywords: quantization, nonholonomic systems, geometric quantization

Introduction

It has been known since 1899 that the dynamics of a mechanical system subject to nonintegrable constraints on the velocities—otherwise known as a *nonholonomic system*—cannot be derived from Hamiltonian's principle [23]. Since nonholonomic systems are not Hamiltonian, it is therefore not possible to employ the standard quantization procedure to study the quantum mechanics of these systems. As a result, past attempts to quantize nonholonomic systems have resorted to a variety of ad hoc techniques that have generally led to poor results (discussed in section 4). In this paper we present a consistent quantization of nonholonomic systems based on the author's prior work in the field of *Hamiltonization*.

Broadly speaking, Hamiltonization employs a variety of techniques to embed a nonholonomic system in a Hamiltonian one (see [11] for a survey of the main techniques). We will restrict our attention to *conditionally variational* nonholonomic systems. Briefly, these are nonholonomic systems whose mechanics coincide with the mechanics of some Hamiltonian system whose initial conditions satisfy the nonholonomic constraints (a more detailed discussion can be found in section 2). The Hamiltonization of these systems was studied in [12], where the associated Hamiltonian system was explicitly constructed for a well-known class of nonholonomic systems called *abelian Chaplygin* systems. Since the particular Hamiltonization approach taken there realizes the mechanics of a nonholonomic system as

Hamiltonian mechanics (with initial data suitably restricted), quantization is immediately possible. However, the generally nonEuclidean configuration spaces of typical nonholonomic systems requires a careful approach to their quantization.

The paper is organized as follows. We begin with a review of nonholonomic mechanics in section 1, followed by a review of conditionally variational nonholonomic systems in sections 2 and 3. In section 4 we summarize the past attempts to quantize nonholonomic systems and their shortcomings, and in section 5 we quantize conditionally variational systems using tools from geometric quantization (reviewed in the appendix). Section 6 then applies of the theoretical framework developed to study the quantum mechanics of several families of conditionally variational systems, along with some specific examples of physical interest.

1. Nonholonomic systems

Let us begin by defining what we will mean by a 'mechanical system' on a smooth manifold.

Definition 1. Let Q be a smooth n-dimensional Riemannian manifold with metric g, and suppose that it is also connected and orientable. By a *mechanical system on Q* we will mean a pair (Q, L), where $L: TQ \to \mathbb{R}$ is a regular Lagrangian of mechanical type: $L = T - V$, where $T: TQ \to \mathbb{R}$ is the kinetic energy given by $T(q, \dot{q}) = \frac{1}{2} g_{ij} \dot{q}^i \dot{q}^j$, $i, j = 1, \ldots, n$ (here g_{ij} are the components of g) and $V: Q \to \mathbb{R}$ is the potential energy (we identify V with its lift to TQ), and is assumed to be a smooth function.

We note that we will adhere to the Einstein summation convention for repeated indices throughout.

Let us now add constraints to our mechanical system. Suppose that we now define a *constraint distribution* $\mathcal{D} \subset TQ$ by the one-forms $\{\omega^a\}_{a=1}^k$, $k < n$, as

$$\mathcal{D} = \{v \in TQ | \omega^a(v) = 0, \ a = 1, \ldots, k\}. \tag{1.1}$$

We will assume that the constraints are linear and homogeneous, so that locally $\omega^a(v) = c_j^a(q) \dot{q}^j$, and that $\mathcal{D}$ has constant rank. Then the triple $(Q, L, \mathcal{D})$ is known as a *nonholonomic mechanical system* [4].

Now, suppose that a k-dimensional Lie group G acts freely and properly on Q, so that $\overline{Q} := Q/G$ is a manifold. Let $\mathfrak{g}$ be the Lie algebra of G, and ξ_Q the infinitesimal generator on Q corresponding to $\xi \in \mathfrak{g}$. We assume that its lifted action leaves L and $\mathcal{D}$ invariant, and that at each $q \in Q$, the tangent space $T_q Q$ can be decomposed as

$$T_q Q = \mathfrak{g}_Q \oplus \mathcal{D}_q, \quad \text{where} \quad \mathfrak{g}_Q \Big|_q = \left\{ \xi_Q(q) \Big| \xi \in \mathfrak{g} \right\} \tag{1.2}$$

is the tangent to the orbit through $q \in Q$ ([4] section 2.8). Then we will call $(Q, L, \mathcal{D}, G)$ a *Chaplygin nonholonomic system* [4, 6].

Chaplygin systems give rise to a principal bundle $\pi: Q \to \overline{Q}$, with principal connection $\mathcal{A}: TQ \to \mathfrak{g}$ such that $\ker \mathcal{A} = \mathcal{D}$. This connection can then be used to decompose any tangent vector $v_q \in T_q Q$ into horizontal and vertical parts:

$$v_q = \text{hor}(v_q) + \text{ver}(v_q), \tag{1.3}$$

$$\text{where} \quad \text{hor}(v_q) = v_q - \left(\mathcal{A}_q(v_q) \right)_Q(q), \quad \text{ver}(v_q) = \left(\mathcal{A}_q(v_q) \right)_Q(q).$$

We can now form the reduced velocity phase space TQ/G, and the Lagrangian L induces the reduced Lagrangian $l: TQ/G \to \mathbb{R}$ satisfying $L = l \bigcirc \pi_{TQ}$, where $\pi_{TQ}: TQ \to TQ/G$ is the standard projection. Furthermore, the decomposition (1.3) gives rise to the *reduced constrained Lagrangian* $l_c: T\overline{Q} \to \mathbb{R}$ given by $l_c(r, \dot{r}) := L(q, \text{hor}(\dot{q}))$, where $r = \pi(q)$ and $\dot{r} = T_q\pi(\dot{q})$. Locally, we will write the reduced constrained Lagrangian as

$$l_c(r, \dot{r}) = \frac{1}{2}G_{\alpha\beta}(r)\dot{r}^\alpha\dot{r}^\beta - \overline{V}(r), \tag{1.4}$$

where henceforth Greek indices will range from 1 to $m := \dim \overline{Q} = n - k$, the indices a, b, c will range from 1 to $k = \dim G$, and where $\overline{V}: \overline{Q} \to \mathbb{R}$ is defined by $V = \overline{V} \bigcirc \pi$. Since we will be dealing exclusively with the reduced constrained Lagrangian, we will drop the overbar on V henceforth. The $G_{\alpha\beta}$ are the components of the metric on the reduced space M induced by g according to $G_r(v_r, w_r) := g_q(\text{hor}(v_q), \text{hor}(w_q))$, where $r = \pi(q)$.

In this paper we will deal exclusively with the well-studied subclass where $G = \mathbb{R}^l \times \mathbb{S}^{k-l}$, where $0 \leqslant l \leqslant k$, and such that L is G-invariant. These are called *abelian Chaplygin* nonholonomic systems [6]. Since L is assumed to be G-invariant, we have that $l = L$. We will therefore denote the corresponding reduced constrained Lagrangian l_c by L_c

To arrive at the local equations of motion of an abelian Chaplygin nonholonomic system we pick a local trivialization $Q = \overline{Q} \times G$, coordinatized by $q = (r, s)$. The action of G is given by left translation on the second factor; the equations of motion then consist of a system of second-order ordinary differential equations on $\overline{Q}$, together with a system of first-order constraint equations [4]:

$$\frac{d}{dt}\frac{\partial L_c}{\partial \dot{r}^\alpha} - \frac{\partial L_c}{\partial r^\alpha} = -\left(\frac{\partial L}{\partial \dot{s}^a}\right)^* B_{\alpha\beta}^a\dot{r}^\beta, \tag{1.5a}$$

$$\dot{s}^a = -A_\alpha^a(r)\dot{r}^\alpha. \tag{1.5b}$$

Here the star indicates that we have substituted the constraints (1.5b) into (1.5a) *after* differentiation, and

$$B_{\alpha\beta}^a = \frac{\partial A_\beta^a}{\partial r^\alpha} - \frac{\partial A_\alpha^a}{\partial r^\beta} \tag{1.6}$$

are the components of the curvature of A.

2. Conditionally variational nonholonomic systems

As discussed in the Introduction, the full equations of motion (1.5) cannot be realized as Hamilton's equation for some Hamiltonian H [4, 14, 23] (unless of course $\mathcal{B}_{\alpha\beta}^a = 0$, in which case the system is no longer nonholonomic [4]). However, for certain nonholonomic systems there is an associated *Hamiltonian* system whose Hamiltonian equations reproduce (1.5) provided the initial conditions satisfy the nonholonomic constraints (1.5b). This class of nonholonomic systems was studied in [12] and referred to as *conditionally variational systems*. To find the associated Hamiltonian system we use the following results from [12].

Proposition 1. *([12] Propsitions 3 and 5). Suppose that $(Q, L, \mathcal{D}, G)$ is an abelian Chaplygin system, locally described by (1.5). Then:*

1. *The nonholonomic system (1.5) is conditionally variational if and only if the reduced equations (1.5a) are the Euler-Lagrange equations of L_c.*

2. *Suppose that L and the Lagrangian*

$$L_V(r, \dot{r}, \dot{s}) = L - \frac{\partial L}{\partial \dot{s}^a}\left(\dot{s}^a + A_\alpha^a(r)\dot{r}^\alpha\right) \tag{2.1}$$

are both regular, and denote by H_V the Hamiltonian associated with (2.1). Then the (full) nonholonomic mechanics (1.5) are Hamilton's equations for H_V provided the initial conditions satisfy the nonholonomic constraints.

3. *The property of being conditionally variational is unaffected by the addition of a potential function dependent only on the r variables.*

The first part of this proposition completely determines the class of conditionally variational abelian Chaplygin systems through certain conditions on g and the $A_\alpha^a(r)$. To state these, first define the coefficients $F_{\gamma\alpha\beta}(r) := \left(g_{b\gamma} - g_{ba}A_\gamma^a\right)B_{\alpha\beta}^b$. Then the first part of proposition 1 is equivalent to [12]:

$$F_{\tilde{\alpha}\tilde{\alpha}\beta} = 0, \quad \alpha \neq \beta, \tag{2.2a}$$

$$F_{\alpha\beta\gamma} + F_{\beta\alpha\gamma} = 0, \quad \text{for each } \gamma, \text{ for all } \alpha < \beta, \text{ and with } \alpha, \beta \neq \gamma. \tag{2.2b}$$

Here the notation $\tilde{\alpha}\tilde{\alpha}$ has been introduced to indicate that these repeated indices are not being summed over.

We conclude this section by pointing out that the Lagrangian (2.1) of a conditionally variational nonholonomic system need not be regular. In the event that it is, we will call the system a *regular conditionally variational system*. For the remainder of the paper, when we refer to a 'regular conditionally variational system' we will mean an abelian Chaplygin nonholonomic system that is in addition a regular conditionally variational system.

3. Reproducing the nonholonomic mechanics

Let us briefly review how the associated Hamiltonian system of a regular conditionally variational system reproduces the nonholonomic mechanics (1.5).

Consider a regular conditionally variational nonholonomic system satisfying the hypotheses of proposition 1. The Legendre transform allows us to define the conjugate momenta $p = \partial L_V/\partial \dot{q}$ and the Hamiltonian $H_V : T^*Q \to \mathbb{R}$ through $H_V(q, p) = \dot{q}^i p_i - L_V|_{(q,\dot{q}) \mapsto (q,p)}$. Now, since G is abelian and acts (freely and properly) on Q (by translation on the s variables), it induces an action of G on T^*Q. The associated momentum map $J: T^*Q \to \mathfrak{g}^*$ has components

$$J_a(q, p) = p_a. \tag{3.1}$$

Clearly, H_V is also G-invariant (the s variables are cyclic), and thus from Noether's Theorem [27] it follows that that the p_a are conserved. From (2.1) we have

$$p_a = g_{ab}\left(\dot{s}^a + A_\alpha^a(r)\dot{r}^\alpha\right) = \mu_a \implies \dot{s}^a + A_\alpha^a(r)\dot{r}^\alpha = g^{ab}\mu_b, \tag{3.2}$$

since we have assumed in proposition 1 that L is regular, so that g_{ab} is invertible (here g^{ab} is the inverse matrix of g_{ab}).

We can now reduce the system to one with less degrees of freedom as follows. If $\mu \in \mathfrak{g}^*$ is a regular value of J, then the *reduced space* $J^{-1}(\mu)/G = T^*\overline{Q}$ (recall that $\overline{Q} = Q/G$)[1] [27]. For the zero level set of J, the reduced space $T^*\overline{Q}$ always carries the canonical symplectic

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[1] We also note that since we've assumed the action of G to be free it follows that every $\mu \in \mathfrak{g}^*$ is a regular value of J ([19] proposition 2.2).

form [27]. Moreover, the *reduced Hamiltonian* $h_V: T^*\overline{Q} \to \mathbb{R}$ is defined by

$$h_V \bigcirc \pi_\mu = H \bigcirc i_\mu,$$

where $\pi_\mu: J^{-1}(\mu) \to T^*\overline{Q}$ is the canonical projection and $i_\mu: J^{-1}(\mu) \hookrightarrow T^*Q$ is the inclusion [29]; simply put, h_V is just H_V with $p_a = \mu_a$, $a = 1, \ldots, k$. Therefore, the equations of motion on $T^*\overline{Q}$ are simply the canonical Hamiltonian equations of h_V.

Let us now see how the Hamiltonian mechanics of H_V reproduces (1.5) when the initial data satisfy the constraints.

First, note that the Hamiltonian mechanics of H_V is just the reduced mechanics of h_V together with the conservation laws $p_a = \mu_a$. Now, if the initial data (r^0, s^0) satisfy the non-holonomic constraints (1.5b), then the quantities $\dot{s}^a + A_\alpha^a(r)\dot{r}^\alpha$ are all initially zero. It follows from (3.2) that the constants $\mu_a = 0$. Thus, the conservation laws $p_a = 0$ now reproduce (1.5b) via (3.2).

Next, let us describe how the reduced mechanics of h_V reproduce (1.5a). Note that from (3.2) and (2.1) it follows that the Lagrangian l_V associated to h_V is[2]

$$l_V(r, \dot{r}) = L - \frac{\partial L}{\partial \dot{s}^a} g^{ab} \mu_b \mid_{\dot{s}^a = -A_\alpha^a(r)\dot{r}^\alpha - g^{ab}\mu_b}. \tag{3.3}$$

With $\mu_a = 0$ we have $l_V = L_c$, and from the assumption that the system is conditionally variational the first part of proposition 1 gives that (1.5a) is equivalent to the Euler-Lagrange equations for l_V (which are Hamilton's equations for h_V). We will denote the Hamiltonian system associated to a regular conditionally variational system by (Q, H_V, G).

4. Past attempts at quantizing nonholonomic systems

The first known attempt to quantize nonholonomic systems was documented in [9]. There R. Eden quantized nonholonomic systems by first ignoring the nonholonomic constraints and quantizing the nonholonomic system's Hamiltonian H, obtaining a Hilbert space $\mathcal{H}_0$. He then used H to propagate a quantum state $\Psi_0 \in \mathcal{H}_0$ to a state $\tilde{\Psi}_1$, which will in general lie outside of $\mathcal{H}_0$. To enforce the nonholonomic constraints at the quantum level Eden introduced a 'quasi-operator' Q_M to project Ψ_0 back into $\mathcal{H}_0$, so that $\Psi_1 = Q_M \tilde{\Psi}_1 \in \mathcal{H}_0$. He then remarks that 'from the viewpoint of H, the state Ψ_1 appears to have developed from a slightly different initial state from Ψ_0'. His solution is a 'continual adjustment of the apparent initial conditions, such that the equation of constraint remains satisfied'. Unfortunately the paper does not discuss the existence or other properties of the quasi-operator Q_M; his approach was described by the authors of [2] as 'formal and his conclusions qualitative in nature'.

Loosely related to Eden's approach is the work of [28], where a system of two particles on $Q = \mathbb{R}^4$ subject to a nonholonomic constraint was quantized using a projection approach developed by those authors in earlier (cited therein) work. Unfortunately, they reported that 'when canonical quantization is performed, we arrive at an infinite set of inequivalent quantum theories'.

As an alternate approach to the projector line of attack, in [2] the authors quantized two nonholonomic systems—one on $Q_1 = \mathbb{R}^3$ and the other on $Q_2 = \mathbb{R}^2 \times T^2$—by exploiting the fact that both systems are explicitly solvable. Using the trajectories obtained, the authors constructed Hamilton principal functions—solutions to the Hamilton–Jacobi equation—and used them to quantize the systems. Despite their perceived success, at least two drawbacks emerged from the analysis: the approach required the explicit solutions to the dynamics (such

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[2] We note in passing that l_V is the classical Routhian (see [26] proposition 3.6.3).

explicitly integrable systems are rare in both Hamiltonian and nonholonomic mechanics), and no indication was given of how this approach could be generalized to other non-holonomic systems.

Lastly, we mention the recent work of [5]. There the authors coupled a nonholonomic system to an external field and quantized the coupled Hamiltonian system. The approach is promising in theory, however it is not clear how to select the coupling field in general.

5. Quantizing regular conditionally variational systems

The difficulties encountered in quantizing nonholonomic systems can be avoided in the case of conditionally variational systems, as we now show.

In section 3 we showed that the Hamiltonian mechanics of the system (Q, H_V, G) yield the nonholonomic mechanics (1.5) only when given initial data satisfying (1.5b). To study the quantum mechanics of a conditionally variational system we must impose this condition at the quantum level. But since the Hamiltonian mechanics with initial data satisfying (1.5b) is simply the restriction of (Q, H_V, G) to $J^{-1}(0)$, which we will denote by $(Q, H_V, G)_0$, our ultimate goal then is to construct a quantization of $(Q, H_V, G)_0$.

To do so, we will employ various tools from geometric quantization (appendix A contains a brief overview of the subject). We will use the notation introduced there throughout the rest of the paper. With this in mind, let us define precisely what we mean by a quantization of (1.5).

Definition 2. We will say that the abelian Chaplygin regular conditionally variational nonholonomic system (1.5) is quantizable if $(Q, H_V, G)_0$ has a well-defined smooth quantum state space Γ and a well-defined self-adjoint quantum operator on Q on Γ. In this case, we will refer to the nonholonomic system as a quantizable system with associated quantum data (Γ, Q).

We can then prove the following (recall definition 1).

Theorem 1. *Let $(Q, L, \mathcal{D}, G)$ be an abelian Chaplygin regular conditionally variational nonholonomic system, and (Q, L_V) a mechanical system. Denote by g the metric of the kinetic energy term of L_V. Suppose also that*

1. *(Q, g) is a Riemannian manifold that is complete with respect to the metric induced by g;*
2. *The Hamiltonian vector field X_{H_V}, where H_V is the Hamiltonian defined by the Legendre transform of (2.1), is a complete vector field.*

Then $(Q, L, \mathcal{D}, G)$ is quantizable in the Schrödinger representation with associated quantum data Q given by (A.4), Γ defined by

$$\Gamma = \left\{ \psi \in \Gamma_{D^v}\left(L^\omega \otimes N_{D^v}^{1/2} \right) : \ \psi = \psi(r) \right\}. \tag{5.1}$$

Furthermore, the associated Hamiltonian operator Q_{H_V} is given by

$$Q_{H_V} = -\frac{\hbar^2}{2}\left(\Delta - \frac{R}{6} \right) + V, \tag{5.2}$$

where Δ is the Laplace-Beltrami operator and R is the Ricci scalar curvature of the metric g.

Proof. We begin by quantizing the system (Q, H_V, G). Since this is a Hamiltonian system, its quantization (in the Schrödinger representation) via geometric quantization is standard and is outlined in section A.2. The resulting prequantization consists of the quantum state space $\Gamma_{D^v}(L^\omega \otimes N_{D^v}^{1/2})$ of wavefunctions (A.3) together with the quantization map (A.4) and corresponding quantum Hilbert space $\mathcal{H}_{D^v}^{1/2} \cong L^2(Q, \sqrt{\det g})$ (A.6).

To enforce the constraints at the quantum level we require the allowable wavefunctions ψ to satisfy

$$Q_{J_a}(\psi) = 0. \tag{5.3}$$

This may present two problems: (1) the functions J_a may not be quantizable, and (2) the restrictions (5.3) may force the trivial wavefunction to be the only solution.

With regard to the first obstruction, (3.1) shows that the J_a are linear in the momenta and therefore in the space of quantizable functions (section A.2). As for the second obstruction, since G is abelian it follows that $J^{-1}(\mu_a)$ is a coisotropic submanifold of (T^*Q, ω) (here ω is the canonical symplectic form on T^*Q). This is sufficient to guarantee that (5.3) does not automatically yield the trivial solution [19].

Now, from (A.4) and (5.3) we have that

$$0 = Q_{J_a}(\psi) = -i\hbar\frac{\partial\psi}{\partial s^a} \implies \psi(q) = \psi(r). \tag{5.4}$$

Thus, the quantum states that satisfy (5.3) belong to the subspace (5.1). Moreover, the quantum operator (A.4) is self-adjoint for every quantizable function f on T^*Q whose Hamiltonian vector field X_f is complete ([29] proposition 7.1.6).

Finally, since the quadratic-p Hamiltonian H_V does not preserve the vertical polarization, we cannot find the Hamiltonian operator via formula (A.4). However, since we have assumed that X_{H_V} is a complete vector field, X_{H_V} has a global flow ϕ_t and there exists ([22] section 4.5) a sesquilinear pairing $\langle\langle\,,\,\rangle\rangle: \mathcal{H}_{D_t^v}^{1/2} \times \mathcal{H}_{D^v}^{1/2} \to \mathbb{C}$ (the Blattner–Kostant–Sternberg pairing) defined by [3, 22, 31]

$$\langle\langle s_1, s_2\rangle\rangle = \frac{1}{(2\pi\hbar)^{n/2}} \int_{T^*Q} \psi_1\overline{\psi_2} \, (\lambda_1, \lambda_2)\omega^n, \tag{5.5}$$

where $s_i = \psi_i\lambda_i$, with λ_1, λ_2 are half-forms on D^v and $D_t^v = \phi'_t(D^v)$ and (λ_1, λ_2) is the function on T^*Q defined through the isomorphism between the space of half-forms on D_t^v and the space of conjugate half-forms on D^v given by the metaplectic structure on T^*Q [3]. The quantum operator Q_f is then defined by ([29] section 7.2)

$$\left\langle Q_f\tilde{s}, s\right\rangle_{\mathcal{H}_{D^v}^{1/2}} = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\left\langle\langle\phi_t(\tilde{s}), s\rangle\right\rangle. \tag{5.6}$$

For the case of interest here—a mechanical Hamiltonian of the form $H = \frac{1}{2}g^{ij}p_ip_j + V$, where g_{ij} are the components of the Riemannian metric of the kinetic energy of L, and Q is a complete n-dimensional Riemannian manifold—the operator Q_H is given by (5.2) ([31] section 9.7). $\qquad\square$

Remark 1. It is interesting to note that when one studies the problem of constraining a particle to a submanifold of the configuration space (in our terminology this is a *holonomic* constraint) the resulting quantum Hamiltonian again includes an R-correction similar to the one in (5.2) (see [1, 7, 21] and their references), though that of (5.2) arose from the unrelated use of Riemann normal coordinates to calculate (5.6) (see [31] section 7.2 for the details).$\diamond$

Theorem 1 shows that regular conditionally variational systems are quantizable in what is referred to as the *extended phase space quantization* in [19]. Let us now discuss the Hilbert space associated with (5.1).

Theorem 2. *Suppose that G is compact. Then the Hilbert space associated with (5.1) is* $L^2(\overline{Q}, \sqrt{\det g})$.

Proof. The Hilbert space associated with (5.1), which we will denote by $\mathcal{H}_\Gamma$, is the subspace of $\mathcal{H}_{D^\nu}^{1/2}$ defined by

$$\mathcal{H}_\Gamma = \left\{ \psi \in \mathcal{H}_{D^\nu}^{1/2} : \ Q_{J_a}(\psi) = 0 \right\}.$$

We now need to ensure that $\langle \psi, \psi \rangle < \infty$ for $\psi \in \mathcal{H}_\Gamma$. From (A.6),

$$\langle \psi, \psi \rangle = \int_Q \psi(q)\overline{\psi(q)}\sqrt{\det g} \ dq$$
$$= \left(\int_{\overline{Q}} \psi(r)\overline{\psi(r)}\sqrt{\det g} \ dr \right)\left(\int_G ds \right), \tag{5.7}$$

where we have used (5.4). If G is compact the second integral is finite, and since g is independent of s (stemming from the abelian Chaplygin assumption), requiring the first integral to be finite is equivalent to requiring that $\psi(r) \in L^2(\overline{Q}, \sqrt{\det g})$. Thus, $\mathcal{H}_\Gamma \cong L^2(\overline{Q}, \sqrt{\det g})$. (If G is not compact then the Hilbert space $\mathcal{H}_\Gamma$ will consist of distributional wavefunctions.) □

5.1. Checking the hypotheses of theorem 1

In the following section we will be discussing examples of quantizable conditionally variational systems. To check that the hypotheses of theorem 1 are satisfied we will be using the theorem proven below. But first some additional background on Riemannian geometry is needed.

Suppose that (Q, L) is a mechanical system (recall definition 1). Then the connectedness of Q allows the Riemannian metric g on Q to induce a metric space structure on Q in the following way. First, let $p, q \in Q$ and $\gamma : [a, b] \to Q$ be a piecewise differentiable path connecting p and q. Then the length of γ, denoted by $L_g(\gamma)$, is defined by ([8] section 7.2), ([30] section 7.5):

$$L_g(\gamma) = \int_a^b \sqrt{g(\gamma'(t), \gamma'(t))} \ dt. \tag{5.8}$$

Finally, define the distance $d_g(p, q)$ to be the infimum of $L_g(\gamma)$ for all γ connecting p and q. Then (Q, d_g) is a metric space ([8], proposition 7.2.5).

In 1970 Gordon proved that if Q is a complete Riemannian manifold (meaning that (Q, d_g) is a complete metric space) and $V \geqslant 0$ (the potential function of the Lagrangian L) then X_H is a complete vector field [17]. In the examples in the next section $Q = \mathbb{R}^n$ with a nonstandard g, so let us now us these facts, along with some results from linear algebra, to provide sufficient conditions for both completeness of $(\mathbb{R}^n, d_g)$ and completeness of X_H (first, recall definition 1).

Theorem 3. *Let* $(\mathbb{R}^n, L)$ *be a mechanical system and denote by g the Riemannian metric of the kinetic energy of L. Suppose that:*

1. *The eigenvalues of the matrix $g_{ij}(q)$ of g are uniformly bounded both above and below by positive constants (i.e., there exist positive constants a, b such that $a \leqslant \lambda_i(q) \leqslant b$ for all $i = 1, \ldots, n$ and for all $q \in Q$).*
2. *The potential function $V \geqslant 0$ for all $q \in Q$.*

   Then: (1) $(\mathbb{R}^n, d_g)$ is complete, and (2) the Hamiltonian vector field X_H is a complete vector field.

Proof. To prove part (1), fix $q \in \mathbb{R}^n$, and let $v \in T_q\mathbb{R}^n \cong \mathbb{R}^n$. Then $g(v, v)$ is the quadratic form $f(v)$ given by

$$f(v) = g(v, v) = v^T M v,$$

where M is the matrix with components $g_{ij}(q)$ and $v = (v^1, \ldots, v^n)$, where v^i is the ith component of the vector v ([24] section V.7). Now, since g is a Riemannian metric, M is a positive-definite and symmetric matrix. It follows from the principal axes theorem ([25], chapter X, theorem 19) that M is orthogonally diagonalizable, that is, there is an orthogonal matrix Q such that $Q^T M Q = D$, where D is the diagonal matrix of eigenvalues of M. As a consequence, if $\lambda_1(q), \ldots, \lambda_n(q)$ are the eigenvalues of M then in the new variable $y = Q^T v$ (or $v = Qy$) we have

$$f(Qy) = g(Qy, Qy) = y^T Q^T M Q y = y^T D y = \lambda_i(q) y_i^2.$$

Then, from the uniform boundedness assumption we have

$$a\left(y_1^2 + \ldots + y_n^2\right) \leqslant f(Qy) \leqslant b\left(y_1^2 + \ldots + y_n^2\right) \iff a y^T y \leqslant f(Qy) \leqslant b y^T y.$$

In the original variable $v = Qy$ this becomes

$$a v^T v \leqslant f(v) \leqslant b v^T v.$$

But the outer quantities are just multiples of the squared norm of v with respect to the Euclidean metric g_e on $\mathbb{R}^n$. Denoting this norm by $\|v\|_e$ we then have

$$a\left\|v\right\|_e^2 \leqslant f(v) \leqslant b\left\|v\right\|_e^2. \tag{5.9}$$

From the uniform boundedness assumption on a, b it then follows that (5.9) is true for all $q \in Q = \mathbb{R}^n$. Therefore, if we denote by d_{g_e} the distance induced by the Riemannian metric g_e on $T_q Q \cong \mathbb{R}^n$ (the usual Pythagorean distance), then using (5.9) in (5.8) shows that

$$a d_{g_e}(p, q) \leqslant d_g(p, q) \leqslant b d_{g_e}(p, q)$$

for any p, $q \in Q = \mathbb{R}^n$. Thus, every Cauchy sequence in the metric space $(\mathbb{R}^n, d_g)$ is also a Cauchy sequence in the metric space $(\mathbb{R}^n, d_{g_e})$. And because $(\mathbb{R}^n, d_{g_e})$ is complete it follows that $(\mathbb{R}^n, d_g)$ is also complete. Part (2) now follows directly from part (ii) of the theorem in [17]. $\square$

6. Examples

Although the results presented in this paper apply only to conditionally variational non-holonomic systems, this class of systems is quite large. To make this point, in section 6.1 we show how conditionally variational systems can be constructed from Hamiltonian systems, and then in section 6.3 we introduce classes of nonholonomic systems that are automatically conditionally variational. We then study particular examples of each class of systems in sections 6.2.1 and 6.4 and quantize them using theorem 1.

6.1. Constructing conditionally variational systems from Hamiltonian systems

Let (Q_0, L) be a mechanical system and coordinatize Q_0 by r^α, where $\alpha = 1, \ldots, m$. Now enlarge the configuration space to $Q_1 = Q_0 \times \mathbb{R}^l \times \mathbb{S}^{k-l}$, where $0 \leqslant l \leqslant k > 0$, and such that this new space is again a smooth manifold with Riemannian metric $\tilde{g}$ that is independent of s^a—the local coordinates of Q_1/Q_0 (thus $a = 1, \ldots, k$). Denote by $\tilde{L}$ the associated mechanical Lagrangian. Finally, impose the nonholonomic constraints (1.5b), requiring that the $A_\alpha^a(r)$ satisfy two conditions: (1) $B_{\alpha\beta}^a$ are not all zero, and (2) the conditions (2.2a) are satisfied.

　　The above procedure results in a conditionally variational nonholonomic system $(Q_1, \tilde{L}, \tilde{g})$ whose reduced constrained equations of motion (equations (1.5a)) coincide with the Hamiltonian mechanics of the Hamiltonian system $(Q_0, \tilde{L}_c, \hat{g})$, where $\hat{g}$ is determined by $\tilde{g}$ and the components $A_\alpha^a(r)$. By construction, the momenta p_a are conserved. If $\tilde{L}_V$ is regular, then as in section 3 the restriction of the Hamiltonian dynamics of $\tilde{H}_V$ to the zero level sets of the p_a reproduce the constraints (1.5b). In other words, with this procedure one can construct conditionally variational nonholonomic systems from a given Hamiltonian system. In the next section we illustrate this method with an example.

6.2. The 'nonholonomic' two-dimensional oscillator

Let us illustrate the discussion in section 6.1 by starting with a two-dimensional harmonic oscillator system $(\mathbb{R}^2, L)$, where

$$L = \frac{m}{2}\left(4\dot{x}^2 + 5\dot{y}^2\right) - \frac{1}{2}\left(x^2 + y^2\right). \tag{6.1}$$

Here the kinetic energy metric $g = m\,\mathrm{diag}(4, 5)$, where m will soon be seen to be related to the reduced mass of the system.

　　Suppose we now enlarge the configuration space to $Q_1 = Q_0 \times \mathbb{R}^2 = \mathbb{R}^4$, coordinatizing Q_1/Q_0 by (z, w). In the notation of section 1 we have $r = (x, y)$ and $s = (z, w)$. Take the new Lagrangian and constraints to be

$$\tilde{L} = \frac{m}{2}\left(4\dot{x}^2 + 5\dot{y}^2 - \dot{z}^2 - \dot{w}^2\right) - \frac{1}{2}\left(x^2 + y^2\right), \tag{6.2a}$$

$$\dot{z} = (\cos x)\dot{y}, \quad \dot{w} = (\sin x)\dot{y}. \tag{6.2b}$$

　　By comparing the system (6.2) with (1.5) we see that the nonholonomic system (6.2) is an abelian Chaplygin nonholonomic system, where $G = \mathbb{R}^2$. Moreover, since the new metric $\tilde{g} = m\,\mathrm{diag}(4, 5, -1, -1)$ is invertible, $\tilde{L}$ is a regular Lagrangian.[3]

　　Now, since $g_{ab} = -m\,\mathrm{diag}(\delta_{ab})$ and $A_y^z(x) = -\cos x$ and $A_y^w(x) = -\sin x$, a simple calculation show that the right-hand side of (1.5a) is zero, and thus by proposition 1 the system is conditionally variational. Thus (6.2) is an abelian Chaplygin regular conditionally variational nonholonomic system.

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[3]　The equations of motion (1.5) of this nonholonomic system are

$$\ddot{x} = 0, \quad \ddot{y} = 0, \quad \dot{z} = (\cos x)\dot{y}, \quad \dot{w} = (\sin x)\dot{y},$$

where the first two equations ($\ddot{x} = \ddot{y} = 0$) are the reduced equations of motion. The resulting trajectories are either spirals (when $\dot{x}_0 \neq 0$) or lines (when $\dot{x}_0 = 0$).

The constrained Lagrangian of (6.2) is

$$\tilde{L}_c = \frac{4\,m}{2}\left(\dot{x}^2 + \dot{y}^2\right) - \frac{1}{2}\left(x^2 + y^2\right) = \frac{\mu}{2}\left(\dot{x}^2 + \dot{y}^2\right) - \frac{1}{2}\left(x^2 + y^2\right),$$

where the metric is now $\hat{g} = \mu\text{diag}(1, 1)$ and $\mu = 4\,m$. Thus, the reduced constrained mechanics of (6.2) is that of a two-dimensional harmonic oscillator with reduced mass μ. For this reason, we will call the nonholonomic system (6.2) the *nonholonomic two-dimensional oscillator*. Moreover, this discussion serves to illustrate the construction in section 6.1; we have constructed an abelian Chaplygin conditionally variational nonholonomic system from the Hamiltonian system (6.1).

6.2.1. Quantizing the nonholonomic two-dimensional oscillator. Let us now check that the theorem 1 applies to the system (6.2). The associated Lagrangian (2.1) is a special case of ([12] equation (5.3)), and is

$$\widetilde{L}_V = \frac{m}{2}\left(4\dot{x}^2 + 5\dot{y}^2 + \dot{z}^2 + \dot{w}^2 - 2\dot{y}\left(\dot{z}\cos\,x + \dot{w}\sin\,x\right)\right) - \frac{1}{2}\left(x^2 + y^2\right). \tag{6.3}$$

We now need to check that $(Q_1, \tilde{L}_V)$ is a mechanical system in the sense of definition 1, and that the other two items of theorem 1 hold.

To see that $(Q_1, \tilde{L}_V)$ is a mechanical system, note that $Q_1 = \mathbb{R}^n$ is connected and orientable, and the potential energy of $\tilde{L}_V$ is clearly a smooth function. It remains to check that (Q_1, g) is a Riemannian manifold, where g is the metric of the kinetic energy of $\tilde{L}_V$ and that $\tilde{L}_V$ is a regular Lagrangian.

$$\left(g_{ij}\right) = m\begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 5 & -\cos x & -\sin x \\ 0 & -\cos x & 1 & 0 \\ 0 & -\sin x & 0 & 1 \end{pmatrix}. \tag{6.4}$$

This is clearly a symmetric matrix. It is also positive-definite, as we now show. By Sylvester's criterion ([20] theorem 7.2.5), it suffices to show that the determinants of all four upper left submatrices of g are positive. The determinants of the 1×1 and 2×2 submatrices are clearly positive ($m > 0$ since it is one-fourth the reduced mass of the oscillator system). The determinant of the upper 3×3 matrix is

$$m^3\begin{vmatrix} 4 & 0 & 0 \\ 0 & 5 & -\cos x \\ 0 & -\cos x & 1 \end{vmatrix} = 4\,m^3\left(5 - \cos^2 x\right) > 0.$$

Finally, the determinant of g is $16\,m^4 > 0$. Thus, (Q_1, g) is a smooth Riemannian manifold. It follows that g^{-1} exists, making $\tilde{L}_V$ a regular Lagrangian.

Finally, to check the two numbered items of theorem 1 we will apply theorem 3. The eigenvalues of (6.4) are

$$\lambda_1 = \left(3 - \sqrt{5}\right)m, \quad \lambda_2 = m, \quad \lambda_3 = 4\,m, \quad \lambda_4 = \left(3 + \sqrt{5}\right)m.$$

Clearly these are all bounded below by, say, $a = m/10 > 0$ and above by $b = 6\,m > 0$. And since $V \geqslant 0$ (being a sum of squares) theorem 3 applies and thus the two numbered assumptions of theorem 1 hold. We conclude that the nonholonomic two-dimensional oscillator is a quantizable nonholonomic system.

The Hamiltonian of (6.3) is

$$\widetilde{H}_V = \frac{1}{2\mu}\left[p_x^2 + \left(p_y + \left(p_w \sin x + p_z \cos x \right) \right)^2 + 4\left(p_z^2 + p_w^2 \right) \right] + \frac{1}{2}\left(x^2 + y^2 \right), \tag{6.5}$$

and from Mathematica we have

$$R = -\frac{1}{32\mu}, \tag{6.6}$$

so that (5.2) gives

$$\begin{aligned}
Q_{\widetilde{H}_V} = {} & \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - \frac{\hbar^2}{384\mu} + \frac{1}{2}\left(x^2 + y^2 \right) \\
& - \frac{\hbar^2}{2\mu}\left[2\left(\sin x \frac{\partial^2}{\partial y \partial w} + \cos x \frac{\partial^2}{\partial y \partial z} \right) \right. \\
& \left. + \left(\sin x \frac{\partial}{\partial w} + \cos x \frac{\partial}{\partial z} \right)^2 \right] - \frac{2\hbar^2}{\mu}\left[\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial w^2} \right]
\end{aligned} \tag{6.7}$$

with the position and momentum operators are given by (A.2).

In the present case the quantum state space Γ of (5.1) is the space of wavefunctions $\psi(x, y)$, and since $\psi \in \Gamma$ are independent of z and w, when computing $Q_{H_V}(\psi)$ only the first line of (6.7) survives. Thus, writing $\Psi(x, y, t) = \psi(x, y)e^{(i/\hbar)Et}$ the Schrödinger equation becomes

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right] + \frac{1}{2}\left(x^2 + y^2 \right)\psi = \left(E + \frac{\hbar^2}{384\mu} \right)\psi. \tag{6.8}$$

As expected from the discussion in section 6.1, we have obtained the quantum two-dimensional harmonic oscillator system. The subsequent analysis follows the standard treatment of the quantum oscillator (the wavefunction solutions ψ can be found via separation of variables and involve Hermite polynomials). There is, however, an important contribution from the operator formula (5.2): since $R \neq 0$ and is constant (6.8) suggests that the energy levels are shifted down by $\hbar^2/(384\mu)$. The new energy levels are

$$E_n = \frac{\hbar}{\sqrt{\mu}}(1 + n) - \frac{\hbar^2}{384\mu}, \tag{6.9}$$

where $n = 0, 1, 2, \dots$. E_n retains the same $(n + 1)$-fold degeneracy of the standard bi-harmonic oscillator ([16] section 10.8), but the ground state energy has changed. The new ground state energy is

$$E_0 = \frac{\hbar}{\sqrt{\mu}} - \frac{\hbar^2}{384\mu} = \hbar\left(\frac{384\sqrt{\mu} - \hbar}{384\mu} \right).$$

Lastly, we note that since the symmetry group $G = \mathbb{R}^2$ is not compact, theorem 2 does not apply. Indeed, since $\text{vol}(G)$ is not finite, $\mathcal{H}_\Gamma$ consists only of distributional wavefunctions.

6.3. Classes of conditionally variational systems

Consider an abelian Chaplygin nonholonomic system with Lagrangian and constraints

$$L(r, \dot{r}, \dot{s}) = \frac{1}{2}g_{ij}(r)\dot{q}^i\dot{q}^j - V(r), \quad \dot{s}^a = -A_\alpha^a(r)\dot{r}^\alpha, \tag{6.10}$$

where (Q, L) is a mechanical system and $q = (r, s)$ coordinatizes Q. The following two subclasses of these systems are automatically conditionally variational.

Class I. Suppose that the components of g are such that $g_{a\alpha} = g_{ab}A_\alpha^b$. Then

$$\left(\frac{\partial L}{\partial \dot{s}^a}\right)^* = g_{a\alpha}\dot{r}^\alpha + g_{ab}\dot{s}^b = \left(g_{a\alpha} - g_{ab}A_\alpha^b\right)\dot{r}^\alpha = 0.$$

Therefore, the right-hand side of (1.5a) vanishes and by proposition 1 (6.10) is conditionally variational. A particularly simple example of this is the nonholonomic system on $Q = \mathbb{R}^3$ with Lagrangian and constraints

$$L = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) + xy\dot{z}, \quad \dot{z} = -xy.$$

Nonholonomic systems belonging to Class I have the property that the nonholonomic constraints appear as conserved momenta of the Hamiltonian system associated with L [10]. (For example, in the example above $p_z = \partial L/\partial \dot{z} = \dot{z} + xy$ and is conserved by Noether's Theorem.) For this reason, these systems are sometimes referred to as nonholonomic systems with 'dynamic nonholonomic constraints' [4].

Class II. Suppose that (6.10) has the special form

$$L(r, \dot{r}, \dot{s}) = \frac{1}{2}\left(g_{\alpha\beta}(r)\dot{r}^\alpha\dot{r}^\beta + g_{ab}(r)\dot{s}^a\dot{s}^b\right) - V(r) \quad \dot{s}^a = -A_2^a\left(r^1\right)\dot{r}^2.$$

Here the only nonzero curvature component is $B_{12}^a = \partial A_2^a/\partial r^1$, and the right-hand side of (1.5b) is

$$g_{ab}(r)A_2^b\left(r^1\right)\frac{\partial A_2^a}{\partial r^1}\left(\dot{r}^2\right)^2.$$

If we now require that $g_{ab}A_2^b(r^1)$ is nonzero for at least one a-value, then these systems fall outside the first class considered previously. However, requiring the coefficient of $\left(\dot{r}^2\right)^2$ to be zero will still yield a conditionally variational system. In particular, when $g_{ab} = g_a\text{diag}(\delta_{ab})$ then

$$g_a(r)A_2^a\left(r^1\right)\frac{\partial A_2^a}{\partial r^1} = \frac{\partial}{\partial r^1}\left[\frac{1}{2}g_a\left(A_2^a\right)^2\right].$$

We conclude that when the sum on the right-hand side is constant,

$$g_a\left(A_2^a\right)^2 = const, \tag{6.11}$$

where we require at least one product to be nonzero, the system will be conditionally variational.

6.4. A class of quantizable nonholonomic systems

Consider the nonholonomic system with configuration space $Q = \mathbb{R}^4$ and Lagrangian and constraints

$$L = \frac{1}{2}\left(F(x)\dot{x}^2 + G(y)\dot{y}^2 - \dot{z}^2 - \dot{w}^2\right) - V(x, y), \tag{6.12a}$$

$$\dot{z} = a(\cos x)\dot{y}, \quad \dot{w} = a(\sin x)\dot{y}, \tag{6.12b}$$

where $a > 0$ and we impose the following requirements:

1. $F(x)$ and $G(y)$ are smooth functions;
2. There exist constants B and C such that $3a^2 < F(x) < B$ and $4a^2 < G(y) < C$;
3. $V(x, y) \geqslant 0$ and is also smooth.

We will now show that theorem 1 applies and discuss the quantization of (6.12).

To begin, note that (6.12) is an abelian Chaplygin nonholonomic system. Moreover, since $g_{ab} = -\text{diag}(1, 1)$, $A_x^z = -a \cos y$, and $A_x^w = -a \sin y$, and this satisfies (6.11), it follows that (6.12) is a Class II system (cf section 6.3) and is thus conditionally variational. And finally, since the metric of L is invertible we conclude that the system (6.12) is an abelian Chaplygin regular conditionally variational system.

The L_V Lagrangian from (2.1) is

$$L_V = \frac{1}{2}\left(F(x)\dot{x}^2 + G(y)\dot{y}^2 + \dot{z}^2 + \dot{w}^2 - 2a\dot{y}\left(\dot{z}\cos x + \dot{w}\sin x\right)\right) - V(x, y). \tag{6.13}$$

From the assumptions on F and G it follows that the metric of the kinetic energy of L_V is again positive definite (as can be checked by Sylvester's criterion), and so (Q, L_V) is a mechanical system (in the sense of definition (1)). The eigenvalues of the metric g of (6.13) are

$$\lambda_1(q) = 1, \quad \lambda_2(q) = F(x), \quad \lambda_{3,4}(q) = \frac{1 + G(y) \pm \sqrt{16a^2 + (G(y) - 1)}}{2},$$

and are uniformly bounded both above and below by positive constants due to the assumptions made on F and G. Therefore, theorem 3 applies and we conclude from theorem 1 that this class of nonholonomic systems is quantizable.

In the present case the quantum state space Γ of (5.1) is the space of wavefunctions $\psi(x, y)$, and thus when computing $Q_{H_V}(\psi)$ once again only derivatives with respect to x and y survive. The R-correction in this case is

$$R = -\frac{4a^2}{2F(x)\left(G(y) - 4a^2\right)}. \tag{6.14}$$

Thus, the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2}\left[\frac{1}{F(x)}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{G(y)}\frac{\partial^2\psi}{\partial y^2}\right] + \frac{1}{2}\left[V(x, y) - \frac{a^2\hbar^2}{3F(x)\left(G(y) - 4a^2\right)}\right]\psi = E\psi. \tag{6.15}$$

In general this is not a separable equation. We are therefore not able to explicitly study the energy spectrum in general, as we did in example (6.2.1).

However, there are particular cases where more can be said. For example, if $V(x, y) = \frac{1}{2}(x^2 + y^2)$ and we take $F(x) = 4a^2$ and $G(y) = 4a^2 + e^{-y^2}$ (which satisfy the conditions given at the onset of this section), then (6.15) is separable. Writing $E = E_x + E_y$ we obtain

$$-\frac{\hbar^2}{8a^2}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}x^2 = E_x, \quad -\frac{\hbar^2}{2\left(4a^2 + e^{-y^2}\right)}\frac{1}{\psi}\frac{\partial^2\psi}{\partial y^2} + \left[\frac{1}{2}y^2 - \frac{\hbar^2}{24}\right] = E_y.$$

The first equation is easily solvable, but the second is not. Nonetheless, for x, y restricted to a bounded interval and after imposing appropriate initial conditions both of these differential equations can be viewed as regular Sturm–Liouville problems, from which it would follow that the eigenvalues (E_x, E_y in this case) are real ([15] theorem 3.9).

7. Conclusion

We have developed a quantization procedure for abelian Chaplygin regular conditionally variational systems that specifies the quantum state space, operator, and Hilbert space through theorems 1 and 2. The results are based on various tools from the field of geometric quantization and on the properties of conditionally variational nonholonomic systems studied in [12]. While our results do not apply for all nonholonomic systems, as sections 6.1 and 6.3 show the class of conditionally variational nonholonomic systems is large enough to provide a rich set of examples of nonholonomic systems that are now quantizable in a well-defined manner. This is illustrated by the family of quantizable systems studied in section 6.4.

The nonholonomic oscillator example of section 6.2.1 is especially noteworthy. It illustrates the discussion in section 6.1 and also contains new insights into the quantum mechanics of nonholonomic systems. In that example, the R-correction resulting from the operator for the associated Hamiltonian can be interpreted as a shift in the ground state energy of the system. What's more, the following two observations are worthy of mentioning.

Firstly, it is interesting to note that the energy shift caused by the R-correction is absent in the energy levels for the standard two-dimensional quantum harmonic oscillator, despite that system having the same configuration space Q_1 as the conditionally variational system studied in section 6.2. The difference is of course in the Hamiltonians. Since the R-correction is determined by the metric of (6.5), which itself is defined in part by the nonholonomic constraints through (2.1), this suggests that in this example the *quantum* energy correction arises in part from the *classical* nonholonomic constraints.

Secondly, we note that the R-correction (6.6) depends inversely on the reduced mass μ. This suggests that for large μ this correction disappears, in agreement with the fact that no such R-correction is present in the classical dynamics of the nonholonomic system (6.2). The μ-dependency also suggests that an experiment (or quantum simulation) could potentially test for the presence of the R-correction (6.6). This and other physical ramifications of the theory developed herein are currently being investigated in [13].

Acknowledgments

Appendix A. Geometric quantization

We present here a brief review of geometric quantization. The primary sources for the content discussed are [19, 29, 31, 33], each of which offer a thorough exposition of the subject.

A.1. Quantization of Euclidean spaces

Mathematically, the objective of quantization is to associate to a phase space M a Hilbert space $\mathcal{H}$ of quantum states and to smooth functions f on M self-adjoint operators Q_f on $\mathcal{H}$ satisfying certain properties. This is referred to as a *prequantization*. In the simplest case when $M = T^*\mathbb{R}^n$ with the canonical symplectic form $\omega = \mathrm{d}p_i \wedge \mathrm{d}q^i$ (here $1 \leqslant i \leqslant n$), we have the definition of Van Hove ([29] definition 6.1.2):

Definition 3. Let M be a smooth manifold. A prequantization of (M, ω) is a map taking smooth functions $f \in C^\infty(M, \mathbb{R})$ to self-adjoint operators Q_f on a Hilbert space $\mathcal{H}$ satisfying the 'Dirac conditions'

1. $Q_{f+g} = Q_f + Q_g$, for each $f, g \in C^\infty(M, \mathbb{R})$,
2. $Q_{\lambda f} = \lambda Q_f$, for each $f \in C^\infty(M, \mathbb{R})$ and $\lambda \in \mathbb{R}$,
3. $Q_{1_{\mathbb{R}^n}} = \mathrm{Id}_{\mathcal{H}}$,
4. $[Q_f, Q_g] = (Q_f \bigcirc Q_g - Q_g \bigcirc Q_f) = i\hbar Q_{\{f,g\}_\omega}$, for each $f, g \in C^\infty(M, \mathbb{R})$,

where $\{f, g\}_\omega$ is the Poisson bracket of f and g and $\hbar = h/2\pi$, where h is Planck's constant.

In [32] Van Hove proved that

$$Q_f = -i\hbar X_f - \theta\left(X_f\right) + f, \quad \text{where} \quad \theta = p_i \, dq^i,$$

where X_f is the Hamiltonian vector field of the function $f \in C^\infty(T^*\mathbb{R}^n, \mathbb{R})$, gives a prequantization of $(T^*\mathbb{R}^n, \omega)$ with $\mathcal{H} = L^2(\mathbb{R}^n)$.

A.2. Quantization of cotangent bundles

If $Q \neq \mathbb{R}^n$, care must be taken in the quantization scheme used. Let us now give a brief overview of geometric quantization, which provides a quantization scheme in this case. As stated in [22], the basic ingredients are: (1) a symplectic manifold, (2) a prequantization of it with a connection ∇ with a Hermitian structure on the fibers, (3) a polarization, and (4) a metaplectic structure.

Let us begin by taking the cotangent bundle with its canonical symplectic structure, $(T^*Q, \omega = \mathrm{d}\theta)$. Since ω is exact it represents an integral cohomology class (its cohomology class is zero). Therefore, (T^*Q, ω) is said to be *quantizable*. Following ([29] chapters 6–8), we can then construct a prequantization of (T^*Q, ω) as follows.

First, the condition on ω guarantees the existence of a complex line bundle $L^\omega = (T^*Q \times \mathbb{C}, \pi, T^*Q)$ over T^*Q. Denoting by $\Gamma(L^\omega)$ the sections[4] of L^ω, it follows that $\Gamma(L^\omega) \cong C^\infty(T^*Q, \mathbb{C})$. Therefore, our wavefunctions depend on both q and p.

Next, we define a connection on L^ω as follows: for each $X \in \mathcal{X}(T^*Q, \mathbb{C})$ there exists an operator $\nabla_X^\omega : \Gamma(L^\omega) \to \Gamma(L^\omega)$ such that

$$\nabla_X^\omega \psi = X(\psi) - \frac{i}{\hbar}\theta(X)\Psi$$

for each $\psi \in \Gamma(L^\omega)$. This operator is in fact a connection on L^ω with curvature $-i\hbar^{-1}\omega$. We will defer the discussion of the Hermitian structure to section A.3.

Now, to recover the Schrödinger representation we introduce the *vertical distribution*, the distribution $D^v \subset T^*Q$ defined by

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[4] These sections are the *wavefunctions*.

$$D^v = \mathrm{span}\left\{ \frac{\partial}{\partial p_1}, \ldots, \frac{\partial}{\partial p_n} \right\}.$$

The vertical distribution is an involutive n-dimensional distribution on T^*Q such that $(D^v)^\perp = D^v$; such distributions are known as *real polarizations*. Moreover, since $T^*Q/D^v \cong Q$, D^v is a *reducible* real polarization. Denoting by $\Gamma_{D^v}(L^\omega)$ the space of all smooth sections $\psi \in \Gamma(L^\omega)$ such that $\nabla^\omega_X \psi = 0$ for each $X \in \mathcal{X}(T^*Q, D^v)$[5] (i.e. the space of sections constant along the fibers of T^*Q) it follows that $\Psi \in \Gamma_{D^v}(L^\omega)$ if and only if

$$\frac{\partial \psi}{\partial p_i} = 0, \quad i = 1, \ldots, n.$$

Thus $\Gamma_{D^v}(L^\omega) \cong C^\infty(Q, \mathbb{C})$. This recovers the solely q-dependent wavefunctions of the Schrödinger representation.

In order to appreciate the need for the last ingredient for quantization—the metaplectic structure—we now describe the quantum operator $\left(Q_{D^v}\right)_f$. We begin by defining the *space of quantizable functions* on T^*Q in the vertical polarization, denoted by $C^\infty(T^*Q, D^v; \mathbb{R})$, as the subspace of $C^\infty(T^*Q, \mathbb{R})$ given by

$$f \in C^\infty\left(T^*Q, D^v; \mathbb{R}\right) \quad \text{if and only if} \quad \left[X_f, \partial_p\right] \in \mathcal{X}\left(T^*Q, D^v\right).$$

This condition implies that $\partial^2 f / \partial p_i^2 = 0$, or that $f = a_0(q) + a_i(q)p_i$. Therefore, the functions that preserve the vertical polarization are at most linear in p. For $f \in C^\infty(T^*Q, D^v; \mathbb{R})$ the operator $\left(Q_{D^v}\right)_f$ is then given by

$$\left(Q_{D^v}\right)_f = -i\hbar \, \nabla^\omega_{X_f} + f = -i\hbar a_i(q)\frac{\partial}{\partial q^i} + a_0(q), \tag{A.1}$$

and is self-adjoint if X_f is a complete vector field.

The construction (A.1) recovers the familiar Schrödinger operators for q and p:

$$\left(Q_{D^v}\right)_{q^i} = q^i, \qquad \left(Q_{D^v}\right)_{p_i} = -i\hbar\frac{\partial}{\partial q^i}. \tag{A.2}$$

However, it fails to give the correct quantized energies for the one-dimensional harmonic oscillator ([29] example 7.1.8). This issue is resolved by the *half-forms correction*, which consists of extending the structure group of T^*Q from the symplectic group $Sp(2n, \mathbb{R})$ to the metaplectic group $Mp(2n, \mathbb{R})$, the connected double covering of $Sp(2n, \mathbb{R})$. The sections of this bundle are called the *half-forms normal to the polarization*. We now briefly describe this correction (more thorough treatments can be found in ([29] section 7.2 and [22]).

First, denote by K^v_D the (trivial) line bundle over T^*Q generated by $dq^1 \wedge \ldots \wedge dq^n$ and by $N^{1/2}_{D^v}$ the square root of K^v_D; it is generated by $(dq^1 \wedge \ldots \wedge dq^n)^{1/2}$, and so is trivial. We then replace L^ω by $L^\omega \otimes N^{1/2}_{D^v}$. It follows that

$$\Gamma_{D^v}\left(L^\omega \otimes N^{1/2}_{D^v}\right) = \left\{ \psi(q)\left(d^n q\right)^{1/2} : \psi \in C^\infty(Q, \mathbb{C}) \right\}, \tag{A.3}$$

The new operator $Q^{1/2}_{D^v}$ is different from (A.1): first, we define the matrix A whose components are found from

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[5] Here $\mathcal{X}(T^*Q, D^v) = \{X \in \mathcal{X}(T^*Q) : X(x) \in D^v_x \quad \forall \ x \in T^*Q\}$.

$$\left[X_f, \frac{\partial}{\partial p_i} \right] = \sum_{j=1}^{n} a_{ij} \frac{\partial}{\partial p_j}.$$

For $f \in C^\infty(T^*Q, D^\nu; \mathbb{R})$ we have $a_{ij} = \partial a_i / \partial q^j$. The new operator is then given by

$$\left(Q_{D^\nu}^{1/2} \right)_f = -i\hbar \nabla_{X_f}^\omega + f - \frac{1}{2} i\hbar \ tr (A) = -i\hbar a_i(q) \frac{\partial}{\partial q^i} + a_0(q) - \frac{1}{2} i\hbar \sum_{i=1}^{n} \frac{\partial a_i}{\partial q^i}. \qquad (A.4)$$

A.3. The quantum Hilbert spaces

To arrive at the quantum Hilbert space, we first construct a Hermitian structure on L^ω. Consider first an open cover $\mathcal{U} = \{ U_i : i \in I \}$ of T^*Q and introduce the local trivialization

$$\rho_i \colon \pi^{-1}\left(U_i \right) \to U_i \times \mathbb{C}$$

of L^ω, where $\pi \colon L \to M$. We can then construct a Hermitian structure on the fibers of L^ω as follows ([29] section 6.2). Let $l_1, l_2 \in \pi^{-1}(x)$, so that $\rho_i(l_j) = (x, z_j)$ (for $j = 1, 2$ and $i \in I$), and then take $(l_1, l_2)_x = \bar{z}_1 z_2$. This Hermitian structure is compatible with the connection ∇^ω.

Now, for $s, t \in \Gamma_{D^\nu}(L^\omega)$, the smooth complex-valued function (s, t) defined by

$$(s, t) \colon \ x \in T^*Q \mapsto (s(x), t(x))_x \in \mathbb{C}$$

can be seen as a function on Q. Introducing now the inner product

$$\langle s, t \rangle = \int (s, t) d^n q, \qquad (A.5)$$

we define the *pre-Hilbert space* $P\mathcal{H}_{D^\nu}$ by

$$P\mathcal{H}_{D^\nu} = \left\{ s \in \Gamma_{D^\nu}\left(L^\omega \right) \colon \ \langle s, s \rangle < \infty \right\}.$$

Then the quantum Hilbert space $\mathcal{H}_{D^\nu}$ is the completion of $P\mathcal{H}_{D^\nu}$ with respect to the inner product (A.5). Since the $s \in \Gamma_{D^\nu}(L^\omega)$ are independent of p, we have that $\mathcal{H}_{D^\nu} \cong L^2(Q)$.

To define the quantum Hilbert space after the half-forms correction, we first define the inner product by [18]

$$\left\langle \psi_1(q)\left(d^n q \right)^{1/2}, \psi_2(q)\left(d^n q \right)^{1/2} \right\rangle = \int \psi_1(q) \overline{\psi_2(q)} \sqrt{\det g} \ d^n q. \qquad (A.6)$$

The corresponding quantum Hilbert space $\mathcal{H}_{D^\nu}^{1/2} \cong L^2(Q, \sqrt{\det g})$, the Hilbert space of complex-valued functions on Q that are square integrable with respect to the density $\sqrt{\det g}$ [18, 31].

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