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Geometric Generalisations of SHAKE and RATTLE

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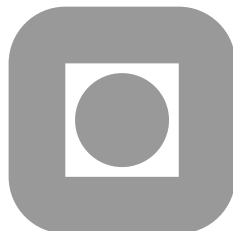
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Geometric Generalisations of SHAKE and RATTLE

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A geometric analysis of the SHAKE and RATTLE methods for constrained Hamiltonian problems is carried out. The study reveals the underlying differential geometric foundation of the two methods, and the exact relation between them. In addition, the geometric insight naturally generalises SHAKE and RATTLE to allow for a strictly larger class of constrained Hamiltonian systems than in the classical setting.

In order for SHAKE and RATTLE to be well defined, two basic assumptions are needed. First, a nondegeneracy assumption, which is a condition on the Hamiltonian, i.e., on the dynamics of the system. Second, a coisotropy assumption, which is a condition on the geometry of the constrained phase space. Non-trivial examples of systems fulfilling, and failing to fulfill, these assumptions are given.

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1 Introduction

SHAKE and RATTLE are two commonly used numerical integration methods for Hamiltonian problems subject to holonomic constraints [16, 1, 11, 9, 15]. The difference between the two methods is that RATTLE preserves “hidden” constraints, whereas SHAKE does not. For details and a historical account, see the monographs [10, § 7.2] and [8, § VII.1.4].

In this paper we give a rigorous geometric analysis of the SHAKE and RATTLE methods. Our approach is based on an observation by Reich [15], that SHAKE and RATTLE may be expressed using flow maps. The analysis sheds light on the underlying “geometric foundation” of the two methods, and also on the exact relation between them. In addition, the geometric insight allows us to integrate a larger class of constrained problems than before. Indeed, the geometric versions of SHAKE and RATTLE work for *coisotropic constraints*. This class of constraints is strictly larger than the class of holonomic constraints. In particular, they may depend on both position and momentum.

Throughout the paper we utilise the language of differential geometry. The main reason for doing so is *not* to generalise SHAKE and RATTLE from \mathbf{R}^{2d} to manifolds, but rather because this notation makes the geometric structures more transparent. However, in order to link to the standard literature on SHAKE and RATTLE, we give many key results also in the classical \mathbf{R}^{2d} setting as examples.

Our notation closely follows that of Marsden and Ratiu [13]. In particular, if \mathcal{M} and \mathcal{N} are two manifolds and $f \in \mathcal{C}^\infty(\mathcal{M}, \mathcal{N})$, then $\mathbb{T}f: \mathbb{T}\mathcal{M} \rightarrow \mathbb{T}\mathcal{N}$ denotes the tangent derivative. If $\mathcal{N} \subset \mathcal{M}$ is a submanifold, then $\iota_{\mathcal{N}}: \mathcal{N} \rightarrow \mathcal{M}$ denotes the inclusion, and the pullback of differential forms from \mathcal{M} to \mathcal{N} is denoted $\iota_{\mathcal{N}}^*$. If (\mathcal{P}, ω) is a symplectic manifold, and $H \in \mathcal{C}^\infty(\mathcal{P})$, then X_H denotes the corresponding Hamiltonian vector field, and the Poisson bracket is denoted $\{\cdot, \cdot\}$. The contraction between a vector X and a differential form α is denoted $i_X\alpha$.

We continue this section with an outline of the paper and the main results.

Problem formulation Let (\mathcal{P}, ω) be a symplectic manifold, $H \in \mathcal{C}^\infty(\mathcal{P})$ a smooth function, and $\mathcal{M} \subset \mathcal{P}$ a submanifold. Given $(\mathcal{P}, \omega, H, \mathcal{M})$, the problem is to find a smooth curve $t \mapsto \gamma(t)$ such that

$$i_{\mathcal{M}}^*(i_{\dot{\gamma}}\omega - dH) = 0, \quad \gamma(t) \in \mathcal{M}. \tag{1a}$$

Equation (1a) looks like a Hamiltonian system on \mathcal{P} , but constrained to stay on the submanifold \mathcal{M} , called the *constraint manifold*. It can be rewritten as

$$i_{\dot{\gamma}}\nu - dH_{\mathcal{M}} = 0, \tag{1b}$$

where $\nu = i_{\mathcal{M}}^* \omega$ and $H_{\mathcal{M}} = i_{\mathcal{M}}^* H$. From this formulation it is clear that equation (1) is intrinsic to \mathcal{M} , i.e., it only depends on objects defined on \mathcal{M} .

Example 1.1. Let $\mathcal{P} = \mathbf{R}^{2d}$ with canonical coordinates $z = (q, p)$, and let $\mathcal{M} = g^{-1}(\{0\})$, where $g = (g_1, \dots, g_m) \in \mathcal{C}^\infty(\mathbf{R}^{2d}, \mathbf{R}^m)$. Equation (1) then takes the form

$$\begin{aligned} \dot{q} &= H_p(q, p) + g_p(q, p)^\top \lambda \\ \dot{p} &= -H_q(q, p) - g_q(q, p)^\top \lambda \\ 0 &= g(q, p), \end{aligned} \tag{2}$$

where g_q and g_p are the partial Jacobian matrices, and $\lambda = (\lambda_1, \dots, \lambda_m)$ are Lagrange multipliers. Notice that if g does not depend on p , then this reduces to a canonical Hamiltonian system with holonomic constraints.

Owing to the Hamiltonian structure of the equations, the reduction of the differential–algebraic equation (DAE) (2) to an ordinary differential equation (ODE) takes a particular form. This was already noticed by Dirac [2, §1], and later perfected in [4].

Existence and uniqueness Since equation (1) is intrinsic to \mathcal{M} , it is clear that any condition or assumption for existence and uniqueness should also be intrinsic, so it is enough to investigate existence and uniqueness intrinsically on \mathcal{M} .

The 2–form ν is closed, but in general degenerate, so (\mathcal{M}, ν) is not, in general, a symplectic manifold. Instead, it is a *presymplectic* manifold.

The kernel of ν defines a distribution on \mathcal{M} denoted $\ker \nu$. As detailed in §2.1, the kernel distribution is *integrable*. Thus, for each $z \in \mathcal{M}$, there is a submanifold $\mathcal{K}_z \subset \mathcal{M}$ such that $\mathbb{T}_x \mathcal{K}_z = \ker \nu_x$ for each $x \in \mathcal{K}_z$.

If $\gamma(t)$ is a solution to (1b), then $dH_{\mathcal{M}}(\gamma(t)) \in \omega(\mathbb{T}_{\gamma(t)} \mathcal{M})$. Thus, solutions stay on the *hidden constraint set*, given by

$$\mathcal{M}^H = \{z \in \mathcal{M} : dH_{\mathcal{M}}(z) \in \nu(\mathbb{T}_z \mathcal{M})\}. \tag{3}$$

In particular, a necessary condition for equation (1b) to have a solution is that the initial data fulfils $\gamma(0) \in \mathcal{M}^H$, which is assumed from here on.

As is further explained in §2, a sufficient condition for (local) existence and uniqueness of equation (1b), and hence equation (1), is the following.

Assumption 1 (Nondegeneracy). For any $z \in \mathcal{M}$, the critical points of the function $H_{\mathcal{K}_z} = i_{\mathcal{K}_z}^* H_{\mathcal{M}}$ are nondegenerate.

Example 1.2. For the classical setting in Example 1.1,

$$\mathcal{M}^H = \{z \in \mathbf{R}^{2d} : g_i(z) = 0, X_H(z) \cdot \nabla g_i(z) = 0, i = 1, \dots, m\}$$

and Assumption 1 means that the matrix $g_z(z)^\top H_{zz}(z) g_z(z)$ is invertible for $z \in \mathcal{M}^H$. If g does not depend on p , then this is slightly weaker than the classical assumption that $g_q H_{pp} g_q$ is invertible (see Remark 5.1).

Geometric SHAKE and RATTLE We now define SHAKE and RATTLE geometrically.

Definition 1.3 (Geometric SHAKE). Let φ_h be a method approximating $\exp(hX_H)$. The SHAKE mapping $S_h: \mathcal{M} \ni z_0 \mapsto z_1 \in \mathcal{M}$ is defined implicitly by

$$\varphi_h(y) \in \mathcal{M}, \quad y \in \mathcal{K}_{z_0} \cap O, \quad z_1 = \varphi_h(y),$$

where $O \subset \mathcal{M}$ is a suitable open subset containing \mathcal{M}^H .

Definition 1.4 (Geometric RATTLE). Let φ_h be a method approximating $\exp(hX_H)$. The RATTLE mapping $R_h: \mathcal{M}^H \ni z_0 \mapsto z_1 \in \mathcal{M}^H$ is defined implicitly by

$$z_1 \in \mathcal{K}_{\tilde{z}_1} \cap \mathcal{M}^H, \quad \tilde{z}_1 = S_h(z_0).$$

These are abstract definitions of SHAKE and RATTLE. In order to practically be able to implement them, an implicit definition of \mathcal{M} in terms of constraint functions, and a parameterisation of \mathcal{K}_{z_0} , is needed. This issue is discussed in §4, and is related to Assumption 2 introduced below.

In the holonomic case it is already known that SHAKE and RATTLE essentially yield the same method, since the projection step at the end of RATTLE is “neutralised” by the projection step in SHAKE. This observation is made geometrically precise in §4, where we show that SHAKE and RATTLE are two different representations of the same fiber mapping.

Well-posedness of SHAKE and RATTLE The algebraic equations defining SHAKE and RATTLE can be thought of as discretisations of the original equation (1). However, contrary to the continuous case, the discretised equations are *not* intrinsic to \mathcal{M} . Thus, well-posedness of SHAKE and RATTLE depends on how \mathcal{M} is embedded in \mathcal{P} .

Let $\mathbb{T}\mathcal{M}^\perp$ denote the orthogonal complement of $\mathbb{T}\mathcal{M}$ with respect to the symplectic form ω , i.e., $u \in \mathbb{T}_x\mathcal{M}^\perp$ if and only if $\omega(u, v) = 0$ for all $v \in \mathbb{T}_x\mathcal{M}$.

Definition 1.5. A submanifold \mathcal{M} of \mathcal{P} is called *coisotropic* if $\mathbb{T}\mathcal{M}^\perp \subset \mathbb{T}\mathcal{M}$.

As is explained carefully in §3, the natural assumption in order for SHAKE and RATTLE to be well-posed is the following, which is a completely extrinsic condition, i.e., it only has to do with how \mathcal{M} is embedded in \mathcal{P} .

Assumption 2 (Coisotropy). \mathcal{M} is a coisotropic submanifold of \mathcal{P} .

Example 1.6. For the setting in Example 1.1, let g_1, \dots, g_m be the components of the vector valued constraint function g . Then Assumption 2 means that

$$\{g_i, g_j\}(z) = 0, \quad \forall z \in \mathcal{M}.$$

An equivalent interpretation of Assumption 2 is that none of the Lagrange multipliers in equation (2) are resolved by differentiating the constraint condition once. From a DAE point of view, the nondegeneracy and coisotropy assumptions together asserts that equation (2) has index 3. An important particular case is obtained when g does not depend on p . In that case, Assumption 2 *always holds* (see §5.1). As shown in §3.2, Assumption 2 also implies that \mathcal{K}_z is parameterised by

$$(\lambda_1, \dots, \lambda_m) \mapsto \exp\left(\sum_{i=1}^m \lambda_i X_{g_i}\right)(z).$$

In turn, this means that the geometric SHAKE method is given by

$$S_h = \varphi_h \circ \exp\left(\sum_{i=1}^m \lambda_i X_{g_i}\right)$$

where $\lambda_1, \dots, \lambda_m$ are determined implicitly by the conditions $g_i \circ S_h = 0$. Likewise, the geometric RATTLE method is given by

$$R_h = \exp\left(\sum_{i=1}^m \sigma_i X_{g_i}\right) \circ S_h$$

where $\sigma_1, \dots, \sigma_m$ are determined implicitly by $(X_H \cdot \nabla g_i) \circ R_h = 0$.

It is easy to find instances where the coisotropic and/or the nondegeneracy assumptions do not hold, and where the SHAKE and RATTLE methods are not well-defined. For example, if we take as constraint $H = \text{const}$, then the nondegeneracy assumption does not hold, and it is easy to see that SHAKE and RATTLE are not well-defined. This is expected, since the result by Ge and Marsden [3] asserts that it is not (in general) possible to construct symplectic and energy preserving methods. In § 5.2 we give further examples of failing assumptions. Lastly, in § 5.4 we also give a numerical example of a Hamiltonian problem with mixed position and momentum constraints, where we use the geometric SHAKE and RATTLE methods.

Main results The main results in the paper can be summarised as follows.

1. Under [Assumption 1](#), the set \mathcal{M}^H is a symplectic submanifold with symplectic form $\varpi = i_{\mathcal{M}^H}^* \nu$, and equation (1) is well-posed for initial data in \mathcal{M}^H . ([Theorem 2.7](#))
2. Under [Assumption 1](#) and [Assumption 2](#), there exists an open set $O \subset \mathcal{M}$, containing \mathcal{M}^H , such that the SHAKE map $S_h: O \rightarrow O$ is well defined and presymplectic, i.e., $S_h^* \nu = \nu$. Further, it is convergent of order at least 1. ([Theorem 4.1](#) and [Proposition 4.4](#))
3. Under [Assumption 1](#) and [Assumption 2](#), the RATTLE map $R_h: \mathcal{M}^H \rightarrow \mathcal{M}^H$ is well defined and symplectic, i.e., $R_h^* \varpi = \varpi$. Further, it is convergent of order at least 1. ([Theorem 4.1](#) and [Proposition 4.4](#))

2 Hamiltonian Systems on Presymplectic Manifolds

In this section we investigate the geometric structures of equation (1) from the intrinsic viewpoint, i.e., without “looking outside” of \mathcal{M} .

In general, a *presymplectic manifold* is a pair (\mathcal{M}, ν) , where \mathcal{M} is a smooth manifold, and ν is a closed 2-form on \mathcal{M} called a *presymplectic form*. The difference from a symplectic form is that ν need not be nondegenerate. Thus, a symplectic manifold is a special case of a presymplectic manifold. We review some geometric concepts of presymplectic manifolds that are essential in the remainder. For a more thorough treatment, we refer to the book by Libermann and Marle [12].

Given a function $H_{\mathcal{M}} \in \mathcal{C}^\infty(\mathcal{M})$, equation (1b) constitutes a Hamiltonian system on (\mathcal{M}, ν) . Since ν might be degenerate, this equation is not, in general, an ordinary differential equation, but instead a DAE. We show in § 2.3 that under [Assumption 1](#) it is an index 1 DAE on \mathcal{M} . (In § 3 we take the complementary extrinsic viewpoint, and we show that under [Assumption 1](#) and [Assumption 2](#) equation (1) can be interpreted as an index 3 problem on \mathcal{P} .)

2.1 Foliation

Throughout the paper we make the following “blanket assumption”:

The dimension of the kernel distribution $\ker \nu$ is constant.

One important consequence is that the distribution $\ker \nu$ (now assumed to be *regular*) is *integrable* (cf. [6, Th. 25.2]). That is, at each point $x \in \mathcal{M}$ there is a submanifold $\mathcal{K}_x \subset \mathcal{M}$

passing through x whose tangent spaces coincides with the distribution. The submanifolds \mathcal{K}_x are called *leaves*, and the collection \mathcal{K} of all leaves is called a *foliation*.

Remark 2.1. The foliation defines an equivalence class by $y \in [x]$ if $y \in \mathcal{K}_x$. We denote the set of all such equivalence classes by $\overline{\mathcal{M}}$. The projection is given by

$$\pi: \mathcal{M} \ni x \rightarrow [x] \in \overline{\mathcal{M}}.$$

The set $\overline{\mathcal{M}}$ may or may not be a smooth manifold. When it is, the presymplectic form ν descends to a symplectic form $\bar{\nu}$ on $\overline{\mathcal{M}}$, and π is a symplectic submersion. The projection map π being a submersion means that we have a *fibration* of \mathcal{M} . Locally, every foliation is a fibration, but not necessarily globally.

A *presymplectic mapping* is a mapping $\varphi: \mathcal{M} \rightarrow \mathcal{M}$ that preserves the presymplectic form ν , i.e., for which

$$\nu(u, v) = \varphi^* \nu(u, v) := \nu(\mathbb{T}\varphi \cdot u, \mathbb{T}\varphi \cdot v) \quad \forall u, v \in \mathbb{T}_x \mathcal{M}.$$

There is a certain class of mappings that are trivial in the sense that they reduce to the identity mapping in the quotient manifold $\overline{\mathcal{M}}$.

Definition 2.2. A smooth mapping $\varphi: \mathcal{M} \rightarrow \mathcal{M}$ is called *trivially presymplectic* if it preserves each leaf, i.e., if

$$\varphi(x) \in \mathcal{K}_x \quad \text{for all } x \in \mathcal{M}.$$

The following result is clear.

Proposition 2.3. *If φ is trivially presymplectic, then it is presymplectic.*

2.2 Hidden Constraints

The fact that ν does not have full rank reflects that, in general, the possible solutions of (1b) do not fill the whole manifold \mathcal{M} . Indeed, if a curve $\gamma(t)$ is a solution of (1b), then $dH(\gamma(t))$ must be in the set $\nu(\mathbb{T}_{\gamma(t)}\mathcal{M})$. As already seen in §1, the set of points at which this is fulfilled defines the hidden constraint set $\mathcal{M}^H \subset \mathcal{M}$, given by (3).

Remark 2.4. In general, this set is defined as the locus of m functions, where m is the dimension of \mathcal{K}_x . However, if the differential of those functions are not independent at the locus points, the set \mathcal{M}^H need not be a submanifold, and if it is a submanifold, it need not be of codimension m . For instance, we may have $\mathcal{M}^H = \mathcal{M}$ if the Hamiltonian H is constant along each leaf \mathcal{K}_x . This is in particular the case if ν is nondegenerate.

Remark 2.5. The subset \mathcal{M}^H is, strictly speaking, not a set of *hidden* constraints, but rather *implicit* constraints as a consequence of (1b).

2.3 Nondegeneracy Assumption

In this section we show that the nondegeneracy assumption, [Assumption 1](#), ensures that: (i) \mathcal{M}^H is a submanifold of \mathcal{M} ; (ii) $\varpi = \iota_{\mathcal{M}^H}^* \nu$ is a symplectic form; and (iii) the initial value problem (1b) is a Hamiltonian problem on (\mathcal{M}^H, ϖ) . As a consequence, problem (1b) have unique solutions for initial data in \mathcal{M}^H .

From a DAE point of view, [Assumption 1](#) ensures that the DAE (1b) on \mathcal{M} has index 1. As it turns out (see §4 below), the nondegeneracy assumption, together with [Assumption 2](#), also asserts that the geometrically defined SHAKE and RATTLE methods are well defined.

We start with the observation that \mathcal{M}^H is the set of critical points of $H_{\mathcal{K}_x}$.

Proposition 2.6. For $x \in \mathcal{M}$, let $H_{\mathcal{K}_x} = i_{\mathcal{K}_x}^* H_{\mathcal{M}}$. Then

$$\mathcal{M}^H = \{y \in \mathcal{M} : dH_{\mathcal{K}_x}(y) = 0\}$$

Proof. If $y \in \mathcal{M}^H \cap \mathcal{K}_x$ then $dH_{\mathcal{K}_x}(y) = 0$ since $dH(y) \in \nu(\mathbb{T}_y \mathcal{M})$. Thus, the set $\mathcal{M}^H \cap \mathcal{K}_x$ consists of critical points of the function $H_{\mathcal{K}_x}$. \square

Theorem 2.7. Under *Assumption 1*, the following holds.

1. The set \mathcal{M}^H is a submanifold of \mathcal{M} .
2. At a point $x \in \mathcal{M}^H$ we have

$$\mathbb{T}_x \mathcal{M} = \mathbb{T}_x \mathcal{M}^H \oplus \ker \nu.$$

In particular, the presymplectic form ν restricted to \mathcal{M}^H is a symplectic form. Thus, \mathcal{M}^H is a symplectic manifold.

3. Equation (1b) has unique solutions for initial data in \mathcal{M}^H . These solutions are given by the solutions of the Hamiltonian problem on \mathcal{M}^H obtained by restricting H to \mathcal{M}^H .

Proof. Each statement is proved respectively as follows.

1. Let X_1, \dots, X_m be linearly independent vector fields on M that span the distribution $\ker \nu$. Define the functions $\rho_i(x) := \langle dH(x), X_i(x) \rangle$. Then, using [Proposition 2.6](#),

$$\mathcal{M}^H = \{x \in \mathcal{M} : \rho_i(x) = 0, \quad i = 1, \dots, m\}.$$

\mathcal{M}^H is a submanifold if $d\rho_1(x), \dots, d\rho_m(x)$ are linearly independent for every $x \in \mathcal{M}^H$. An equivalent condition is that the matrix

$$m_{ij} := \langle d\rho_i(x), X_j(x) \rangle, \quad i, j = 1, \dots, m$$

be invertible for every $x \in \mathcal{M}^H$. Using that $\rho_i(x) = 0$, we get in local coordinates x_j that

$$m_{ij} = X_i^\alpha(x) \frac{\partial^2 H(x)}{\partial x^\alpha \partial x^\beta} X_j^\beta(x)$$

where $X_i = X_i^\alpha \frac{\partial}{\partial x^\alpha}$. Since $X_1(x), \dots, X_m(x)$ is a linearly independent basis of $(\ker \nu)_x = \mathbb{T}_x \mathcal{K}_x$, [Assumption 1](#) means exactly that this matrix is invertible, which thus proves the first assertion.

2. For the second assertion, using that the codimension of \mathcal{M}^H is m , it suffices to prove that $(\ker \nu)_x \cap \mathbb{T}_x \mathcal{M}^H = 0$ for every $x \in \mathcal{M}^H$. Let $u \in \mathbb{T}_x \mathcal{M}^H$. Then $\langle d\rho_i(x), u \rangle = 0$. Next, assume that $U \in (\ker \nu)_x$. Then U can be expanded as $U = u^i X_i(x)$. We now get

$$0 = \sum_{i=1}^m u^i \langle d\rho_j, X_i(x) \rangle = m_{ij} u^i.$$

Under [Assumption 1](#) we know that m_{ij} is invertible, which implies that $U = 0$. Thus, $(\ker \nu)_x \cap \mathbb{T}_x \mathcal{M}^H = 0$, which proves that ν restricted to \mathcal{M}^H is nondegenerate.

3. For the final assertion, it is enough to show that $\gamma(t)$ is a solution to equation (1b) if and only if it is a solution to the Hamiltonian problem

$$\nu(\dot{\gamma}(t), U) = \langle dH(\gamma(t)), U \rangle, \quad \forall U \in \mathbb{T}\mathcal{M}^H$$

on the symplectic manifold \mathcal{M}^H (for which existence and uniqueness follows from standard ODE theory). As we have seen, under [Assumption 1](#) every $X \in \mathbb{T}_{\gamma(t)}\mathcal{M}$ can be written $X = U + W$ with $U \in \mathbb{T}\mathcal{M}^H$ and $W \in \ker \nu$. Now,

$$\nu(\dot{\gamma}(t), X) = \nu(\dot{\gamma}(t), U) \quad \text{and} \quad \langle dH(\gamma(t)), X \rangle = \langle dH(\gamma(t)), U \rangle$$

where the first and second equality follows respectively since $W \in \ker \nu$ and

$$\langle dH(\gamma(t)), W \rangle = \left\langle dH(\gamma(t)), \sum_i w^i X_i(\gamma(t)) \right\rangle = \sum_i w^i \rho_i(\gamma(t)) = 0.$$

This ends the proof. \square

Remark 2.8. If the prescribed initial condition does not lie in the set \mathcal{M}^H , there cannot be any solution curve passing through this point. On the other hand, if \mathcal{M}^H is a submanifold, and if it intersects the leaves \mathcal{K} cleanly, i.e., if the dimension of the intersection is constant, and if that dimension is larger than zero, then the equation may have infinitely many solutions. This is what happens if H is constant on the leaves of the foliation \mathcal{K} .

The following result will be useful in [§ 4](#), when we analyse SHAKE and RATTLE.

Corollary 2.9. *Under [Assumption 1](#), there exists an open set $O \subset \mathcal{M}$ containing \mathcal{M}^H such that the equation $y \in \mathcal{K}_x \cap \mathcal{M}^H$ has a unique solution for every $x \in O$. The corresponding trivially presymplectic projection map $\Pi: O \rightarrow \mathcal{M}^H$, defined by $\Pi(x) = y$, is a submersion.*

Proof. This follows from [Theorem 2.7 item 2](#), namely that for $x \in \mathcal{M}^H$, $\mathbb{T}_x\mathcal{M} = \mathbb{T}_x\mathcal{M}^H \oplus \ker \nu$. \square

3 Coisotropic Constraints

In this section we study the geometry of problem (1) from the extrinsic viewpoint. That is, we study properties of \mathcal{M} as a submanifold of the symplectic manifold (\mathcal{P}, ω) . Notice that $\nu := i_{\mathcal{M}}^* \omega$ is a presymplectic form on \mathcal{M} , since $d\nu = di_{\mathcal{M}}^* \omega = i_{\mathcal{M}}^* d\omega = 0$. Thus, any submanifold of a symplectic manifold is automatically a presymplectic manifold.

3.1 Lagrange Multipliers

Typically, a constraint manifold is defined in terms of a number of constraint functions. To this extent, let V be a vector space of dimension m , and denote by V^* its dual. Let $J: \mathcal{P} \rightarrow V^*$ be a smooth function such that the constraint submanifold \mathcal{M} is given by

$$\mathcal{M} = J^{-1}(0) = \{z \in \mathcal{P} : J(z) = 0\}. \quad (4)$$

If 0 is a regular value for J , i.e., if $\mathbb{T}J(z)$ has full rank for all $z \in \mathcal{P}$ such that $J(z) = 0$, then \mathcal{M} is indeed a regular submanifold of \mathcal{P} . The dimension m of V is the number of constraints, i.e., the codimension of \mathcal{M} .

The problem (1) may now be reformulated as finding a smooth curve

$$t \mapsto (z(t), \Lambda(t)) \in \mathcal{P} \times V$$

such that

$$\begin{aligned} \omega(\dot{z}) &= dH(z) + d\langle J, \Lambda \rangle(z), \\ 0 &= J(z). \end{aligned} \tag{5a}$$

Here, the notation $\langle J, \Lambda \rangle$ means the smooth function $z \mapsto \langle J(z), \Lambda \rangle$, depending on the parameter Λ . The equation can equivalently be written as

$$\begin{aligned} \dot{z} &= X_H(z) + X_{\langle J, \Lambda \rangle}(z), \\ 0 &= J(z). \end{aligned} \tag{5b}$$

We sometimes single out a basis $\{e_i\}_{i=1, \dots, m}$ of V and define the functions g_i by

$$g_i(z) := \langle J(z), e_i \rangle. \tag{6}$$

Notice that in the case $\mathcal{P} = \mathbf{R}^{2d}$, equation (5) coincides with equation (2) in Example 1.1 above, with $\lambda = (\lambda_1, \dots, \lambda_m)$ being the coordinate vector of Λ , i.e., $\Lambda = \sum_{i=1}^m \lambda_i e_i$.

The system (5) is again a DAE. Under Assumption 1, it follows from Theorem 2.7 above that this DAE has unique solutions for initial data in \mathcal{M}^H . From a DAE point of view, Assumption 1 asserts that system (5) has index 3.

3.2 Coisotropy Assumption

Due to the solvability result imposed by Assumption 1, the Lagrange multipliers may be resolved as functions of z , which turns equation (5) into

$$\dot{z} = X_H(z) + \sum_{i=1}^m \lambda_i(z) X_{g_i}(z) =: X(z). \tag{7}$$

Notice that $X(z)$ is only defined for $z \in \mathcal{M}^H$ and also that $X(\mathcal{M}^H) \in \mathcal{T}\mathcal{M}^H$, so $X(z)$ defines an ODE on the hidden constraint manifold \mathcal{M}^H . From Theorem 2.7 it follows that its flow is symplectic. However, the individual vector fields $\lambda_i(z) X_{g_i}(z)$ are *not* Hamiltonian vector fields on \mathcal{P} (assuming that $\lambda_i(z)$ is defined also outside of \mathcal{M}^H). In this section we present an assumption on the embedding $\iota_{\mathcal{M}}: \mathcal{M} \rightarrow \mathcal{P}$ which ensures that vector fields of the form $f(z) X_{g_i}(z)$ are trivially presymplectic vector fields on \mathcal{M} . As we will see in § 4, this is essential in order to ensure presymplecticity and symplecticity of SHAKE and RATTLE.

Recall from Definition 1.5 that \mathcal{M} is a *coisotropic* submanifold of \mathcal{P} if $\mathcal{T}\mathcal{M}^\perp \subset \mathcal{T}\mathcal{M}$. Also recall Assumption 2 above (the coisotropy assumption), which states that \mathcal{M} is a coisotropic submanifold. We continue with some consequences of Assumption 2, which are later used in the geometric analysis of SHAKE and RATTLE.

Remark 3.1. It is straightforward to verify that \mathcal{M} being coisotropic is equivalent to $\mathcal{T}\mathcal{M}^\perp$ being *isotropic*, i.e., such that ω restricted to $\mathcal{T}\mathcal{M}^\perp$ is zero.

Remark 3.2. In a sense, a coisotropic submanifold is such that the symplectic form becomes as degenerate as possible (given a fixed number of constraints) when restricted on the submanifold. More precisely, a coisotropic submanifold is such that the dimension of the distribution $\ker \nu$, i.e., dimension of the leaves of \mathcal{K} , is equal to the number of constraints m .

Remark 3.3. From a theoretical point of view, [Assumption 2](#) is not a restriction on the presymplectic manifold \mathcal{M} , since every presymplectic submanifold may be coisotropically embedded in a symplectic manifold [5].

Remark 3.4. In practice as shown in [Proposition 3.5](#), a sufficient condition for the manifold \mathcal{M} defined by the equations $g_i(z) = 0$ for $1 \leq i \leq m$ to be coisotropic is simply that

$$\{g_i, g_j\}(z) = 0, \quad i, j = 1, \dots, m, \quad \forall z \in \mathcal{M}.$$

In particular, if the manifold \mathcal{M} is defined by one constraint, i.e. if $m = 1$, then it is automatically a coisotropic submanifold.

The following result gives alternative characterisations of coisotropic submanifolds.

Proposition 3.5. *Suppose that \mathcal{M} is a submanifold of \mathcal{P} . Then the following conditions are equivalent.*

1. \mathcal{M} is a coisotropic submanifold, i.e., $\mathbb{T}\mathcal{M}^\perp \subset \mathbb{T}\mathcal{M}$.
2. $\ker \nu = \mathbb{T}\mathcal{M}^\perp$

Further, if \mathcal{M} is defined implicitly by (4), then the conditions are also equivalent to

3. For any $\alpha, \beta \in V$, the functions $\langle \mathbb{J}, \alpha \rangle$ and $\langle \mathbb{J}, \beta \rangle$ are in involution on \mathcal{M} , i.e.,

$$\{\langle \mathbb{J}, \alpha \rangle, \langle \mathbb{J}, \beta \rangle\}(z) = 0 \quad \text{for } z \in \mathcal{M}.$$

4. For any $\alpha \in V$, the Hamiltonian vector field $X_{\langle \mathbb{J}, \alpha \rangle}$ is tangent to \mathcal{M} .

In order to prove this, let us start with a lemma concerning the span of the Hamiltonian vector fields $X_{\langle \mathbb{J}, \alpha \rangle}$.

Lemma 3.6. *Define the distribution*

$$\mathcal{O} = \text{span}\{X_{\langle \mathbb{J}, \alpha \rangle}(\mathcal{M}) : \alpha \in V\}.$$

Then $\mathbb{T}\mathcal{M}^\perp = \mathcal{O}$.

Proof. We show that $\mathcal{O}^\perp = \mathbb{T}\mathcal{M}$, which is equivalent to the claim.

$$X \in \mathbb{T}\mathcal{M} \iff \langle d\langle \mathbb{J}, \alpha \rangle, X \rangle = 0 \quad \forall \alpha \in V \iff \omega(X_{\langle \mathbb{J}, \alpha \rangle}, X) = 0 \quad \forall \alpha \in V$$

□

Proof of Proposition 3.5. We do it step by step.

1↔2 In general,

$$\ker \nu = \mathbb{T}\mathcal{M} \cap \mathbb{T}\mathcal{M}^\perp,$$

so $\ker \nu = \mathbb{T}\mathcal{M}^\perp \iff \mathbb{T}\mathcal{M}^\perp \subset \mathbb{T}\mathcal{M}$, and that is the definition of coisotropy of \mathcal{M} .

1↔3 First, for $x \in \mathcal{M}$

$$\{g_i, g_j\}(x) = 0 \iff \omega(X_{g_i}(x), X_{g_j}(x)) = 0,$$

so the functions g_i are in involution on \mathcal{M} if and only if \mathcal{O} (defined in [Lemma 3.6](#)) is isotropic, which is equivalent to \mathcal{M} being coisotropic.

3 \leftrightarrow 4 Finally, it suffices to observe that for a point $x \in \mathcal{M}$,

$$\begin{aligned} X_{\langle J, \alpha \rangle}(x) \in \mathbb{T}_x \mathcal{M} &\iff \langle d\langle J, \beta \rangle, X_{\langle J, \alpha \rangle} \rangle(x) = 0 \quad \forall \beta \in V \\ &\iff \{\langle J, \alpha \rangle, \langle J, \beta \rangle\}(x) = 0 \quad \forall \beta \in V. \end{aligned}$$

□

The following results follows directly from [Lemma 3.6](#) and [Proposition 3.5](#).

Corollary 3.7. *Let $x \in \mathcal{M}$. Then, under [Assumption 2](#), the map*

$$V \ni \alpha \mapsto \exp(X_{\langle J, \alpha \rangle})(x) \in \mathcal{K}_x$$

is a local diffeomorphism. The fibre \mathcal{K}_x is thus locally parametrized by V .

Corollary 3.8. *Let $f \in \mathcal{C}^\infty(\mathcal{P})$ and $\alpha \in V$. Under [Assumption 2](#) the vector field*

$$X(z) := f(z)X_{\langle J, \alpha \rangle}(z)$$

is tangent to \mathcal{M} , and presymplectic when restricted to \mathcal{M} .

3.3 Relation between X_H and \mathcal{M}^H

As a subset of \mathcal{P} , the hidden constraint set \mathcal{M}^H is given by the points on \mathcal{M} where the Hamiltonian vector field X_H is tangential to \mathcal{M} . Let Π denote the projection onto \mathcal{M}^H defined in [Corollary 2.9](#).

Proposition 3.9. *Under [Assumption 2](#), the hidden constraint set \mathcal{M}^H is*

$$\mathcal{M}^H = \{z \in \mathcal{M} : X_H(z) \in \mathbb{T}_z \mathcal{M}\}.$$

Moreover, the differential equation (7) on \mathcal{M}^H can be written

$$\dot{z} = \mathbb{T}_z \Pi \cdot X_H(z).$$

Proof. 1. If $z \in \mathcal{M}^H$, then by definition there exists $Y \in \mathbb{T}_z \mathcal{M}$ such that

$$\langle dH, X \rangle = \omega(Y, X) \quad \forall X \in \mathbb{T}_z \mathcal{M}.$$

Since $\omega(X_H) = dH$, that is equivalent to

$$X_H - Y \in \mathbb{T} \mathcal{M}^\perp.$$

Noticing that [Assumption 2](#) means that $\mathbb{T} \mathcal{M}^\perp \subset \mathbb{T} \mathcal{M}$, and using $Y \in \mathbb{T} \mathcal{M}$ yields $X_H \in \mathbb{T}_z \mathcal{M}$.

2. The differential equation on \mathcal{M}^H is such that

$$\omega(\dot{z}, X) = \langle dH, X \rangle \quad \forall X \in \mathbb{T}_z \mathcal{M}$$

so we obtain

$$\dot{z} - Y \in \mathbb{T}_z \mathcal{M}^\perp,$$

and $\dot{z} = \mathbb{T}_z \Pi \cdot X_H(z)$.

□

Remark 3.10. There are now several ways to compute \mathcal{M}^H . First, without any assumption, one can use the definition (3), and its immediate consequence [Proposition 2.6](#). Under [Assumption 2](#), one can also use [Proposition 3.9](#). If the constraint manifold \mathcal{M} is defined as in (4), a further useful description of \mathcal{M}^H is

$$\mathcal{M}^H = \{z \in \mathcal{M} : \{g_i, H\}(z) = 0 \quad i = 1, \dots, m\}.$$

This follows from the observation that

$$X_H \in \mathbb{T}_z \mathcal{M} \iff \langle dg_i, X_H \rangle = 0, \quad i = 1, \dots, m \quad (8)$$

and $\langle dg_i, X_H \rangle = \{g_i, H\}$.

Based on [Theorem 2.7](#), [Proposition 3.5](#) and [Lemma 3.6](#), we can say much more on the behaviour of X_H in a neighbourhood of \mathcal{M}^H . Indeed, we have the following result, which is a key ingredient in the well-posedness of SHAKE and RATTLE, as will be explained in [§4](#).

Lemma 3.11. *Let $y \in \mathcal{M}^H$ and define the function*

$$\begin{aligned} F: \mathcal{K}_y &\longrightarrow V^* \\ x &\longmapsto dJ(x) \cdot X_H(x). \end{aligned}$$

Then, under [Assumption 1](#) and [Assumption 2](#), the differential of F at y , i.e., the linear mapping

$$dF(y) : \mathbb{T}_y \mathcal{K}_y \longrightarrow V^*,$$

is invertible.

Proof. In terms of the previously introduced basis $\{e_i\}_{i=1, \dots, m}$, the function F is given by

$$F(x) = \sum_{i=1}^m \langle dg_i(x), X_H(x) \rangle e_i = - \sum_{i=1}^m \langle dH(x), X_{g_i}(x) \rangle e_i$$

Under [Assumption 2](#), it follows from [Proposition 3.5](#) and [Lemma 3.6](#) that $X_{g_1}(y), \dots, X_{g_m}(y)$ is a basis for $\mathbb{T}_y \mathcal{K}_y$. Relative to this basis, and the basis $\{e_i\}_{i=1, \dots, m}$ of V , the Jacobian matrix of $dF(y)$ is given by

$$m_{ij} := \langle d \langle dH(y), X_{g_i}(y) \rangle, X_{g_j}(y) \rangle = \{\{H, g_i\}, g_j\}(y)$$

Define $\rho_i(x) := \langle dH(x), X_{g_i}(x) \rangle$. Then $m_{ij} = \langle d\rho_i(y), X_{g_j}(y) \rangle$. Since $y \in \mathcal{M}^H$ we have that $\rho_i(y) = 0$. Now, under [Assumption 1](#) and the exact same argument as in the proof of [Theorem 2.7](#), it follows that m_{ij} is invertible. This concludes the proof. \square

4 Geometry of SHAKE and RATTLE

Geometrically, the basic principle of SHAKE, defined in [Definition 1.3](#), with φ_h as an underlying method, can be described as follows. For some initial data $z \in \mathcal{M}$, slide along the fibre with $z^+ \in \mathcal{K}_z$ such that $\varphi_h(z^+)$ “lands” again on the submanifold \mathcal{M} . The RATTLE method, defined in [Definition 1.4](#), is then a post-processed version of SHAKE, which is described geometrically as follows. For some initial data $z_0 \in \mathcal{M}^H$, take one step with SHAKE landing on $z_1^- \in \mathcal{M}$, then slide along the fiber $\mathcal{K}_{z_1^-}$ to end up on $z_1 \in \mathcal{M}^H \cap \mathcal{K}_{z_1^-}$. This process is visualised in [Figure 1](#).

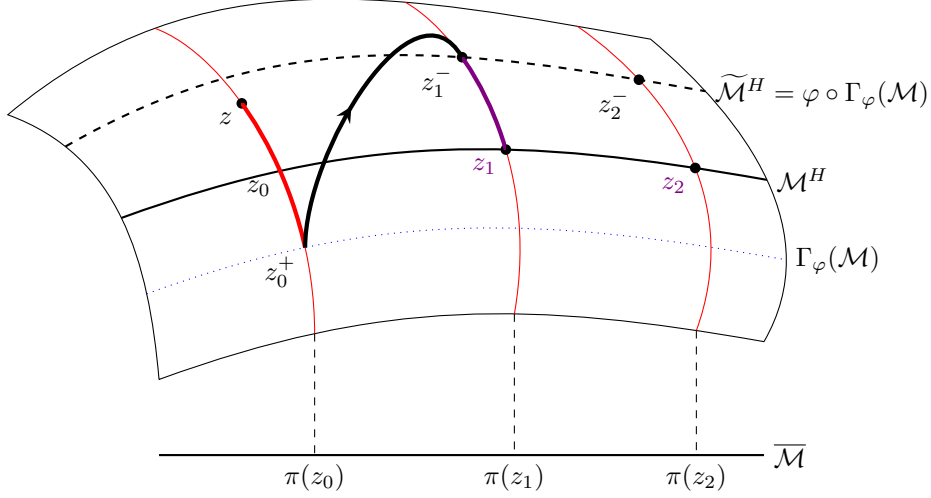


Figure 1: An illustration of the SHAKE and RATTLE method. The first point z must lie in the vicinity of \mathcal{M}^H . The subsequent points z_1^-, z_2^-, \dots produced by SHAKE will all lie in the modified hidden constraint manifold $\widetilde{\mathcal{M}}^H$. The points z_1, z_2, \dots produced by RATTLE will lie on \mathcal{M}^H . Notice how the points z_k^-, z_k and z_k^+ always lie on the same leaf. Moreover, the precise location of a point on the fibre (for instance z on the figure) is irrelevant for both SHAKE and RATTLE.

If we assume that the SHAKE map $S_h: O \rightarrow O$ is well defined for some open subset $O \subset \mathcal{M}$ containing \mathcal{M}^H , then we may define a sliding map $\Gamma_{\varphi_h} = \varphi_h^{-1} \circ S_h$. Consequently, it follows from [Definition 1.3](#) that the sliding map $O \ni z \mapsto \Gamma_{\varphi_h}(z) \in O$ is defined implicitly by the equation

$$\varphi_h(z^+) \in \mathcal{M}, \quad z^+ \in \mathcal{K}_z \cap O, \quad \Gamma_{\varphi_h}(z) = z^+. \quad (9)$$

Notice that: (i) Γ_{φ_h} is fiber preserving, i.e., presymplectic, and (ii) Γ_{φ_h} is a projection, i.e., $\Gamma_{\varphi_h} \circ \Gamma_{\varphi_h} = \Gamma_{\varphi_h}$. Since $S_h = \varphi_h \circ \Gamma_{\varphi_h}$ it follows that SHAKE, if it is well-defined, is a *fiber mapping*, i.e., it maps fibres to fibres. It is, in fact, a little bit more than that, since it maps the whole fibre $\mathcal{K}_z \cap O$ to the same point $S_h(z)$. Hence, when using SHAKE it is not important where on the initial fibre \mathcal{K}_z one starts (as long as it is close enough to \mathcal{M}^H so that SHAKE is well-defined). Furthermore, regardless of where on the fiber one starts, after one step SHAKE remains on the *modified* hidden constraint set, given by

$$\widetilde{\mathcal{M}}^H := \varphi_h \circ \Gamma_{\varphi_h}(O).$$

Since Γ_{φ_h} is a projection, $\widetilde{\mathcal{M}}^H$ is strictly smaller than O . If SHAKE is well-defined, $\widetilde{\mathcal{M}}^H$ is in fact a symplectic submanifold of \mathcal{M} (see [Proposition 4.7](#) below).

Let Π be the projection on \mathcal{M}^H given in [Corollary 2.9](#). Assume that Π is well-defined on O . Then RATTLE is given by $R_h = \Pi \circ S_h$. Notice that SHAKE and RATTLE defined exactly the same fiber mapping. In particular,

$$\Pi \circ (S_h)^k = \Pi \circ (R_h)^k. \quad (10)$$

Thus, RATTLE is only a cosmetic improvement of SHAKE, and has no influence on the numerical scheme except at the last step.

We now give explicit conditions under which SHAKE and RATTLE are well defined and can be computed. More precisely:

1. When is a method φ_h such that the corresponding SHAKE and RATTLE methods are well defined?
2. How can we parameterise Γ_{φ_h} (so that S_h is computable)?
3. Will SHAKE and RATTLE converge to the solution of equation (1) as $h \rightarrow 0$?
4. Are S_h and R_h presymplectic as mappings $O \rightarrow O$?
5. Is R_h symplectic as a mapping $\mathcal{M}^H \rightarrow \mathcal{M}^H$, and S_h symplectic as a mapping $\widetilde{\mathcal{M}}^H \rightarrow \widetilde{\mathcal{M}}^H$?
6. Can S_h or R_h be reversible?

These questions are addressed in the remainder of this section.

4.1 Well-Posedness

In order for SHAKE and RATTLE to be well defined, we need the “sliding process” to have a locally unique solution. Whether so or not depends on the map φ_h .

Theorem 4.1. *Suppose that Assumption 1 and Assumption 2 hold. Consider a (smooth) method φ_h , consistent with $\dot{z} = X_H(z)$. Then for h small enough and for $z \in \mathcal{M}$ in a neighbourhood of \mathcal{M}^H the equation*

$$J(\varphi_h(z^+)) = 0, \quad z^+ \in \mathcal{K}_z \quad (11)$$

has a unique solution.

Proof. Let $x \in \mathcal{M}^H$. We define the function $F_h: \mathcal{K}_x \rightarrow V^*$ by

$$F_h(z^+) := \int_0^1 \frac{\partial}{\partial h} [J(\varphi_h(z^+))] (h\tau) d\tau.$$

We see that F_h depends smoothly on h . Notice that for $h \neq 0$,

$$F_h(z^+) = \frac{J(\varphi_h(z^+)) - J(\varphi_0(z^+))}{h} = \frac{J(\varphi_h(z^+))}{h},$$

because $\varphi_0(z^+) = z^+$ and $z^+ \in \mathcal{M} \iff J(z^+) = 0$.

Consider now the case $h = 0$. The method φ_h is consistent, so $(d\varphi_h/dh)|_{h=0}(z^+) = X_H(z^+)$, which shows that

$$F_0(z^+) = dJ(z^+) \cdot X_H(z^+). \quad (12)$$

We want to find a neighbourhood $O_h \subset \mathcal{K}_x$ of x such that the equation $F_h(z^+) = 0$ with $z^+ \in O_h$ has a unique solution for small enough h . This will prove the claim. The strategy is to show that $dF_h(x): T_x\mathcal{K}_x \rightarrow V^*$ is non-singular. We start with the case $h = 0$.

Using (12) and appealing to Lemma 3.11, $dF_0(x)$ is invertible under Assumption 1 and Assumption 2. Thus, by the inverse function theorem, we can find an open neighbourhood $O_0 \subset \mathcal{K}_x$ such that $F_0: O_0 \rightarrow F_0(O_0)$ is a diffeomorphism. Also, since F_h depends smoothly on h , it follows that $dF_h(x)$ is invertible for small enough h . Thus, for small enough h , we can find an open neighbourhood $O_h \subset \mathcal{K}_x$ such that $F_h: O_h \rightarrow F_h(O_h)$ is a diffeomorphism.

It remains now to show that $0 \in F_h(O_h)$, so that the equation $F_h(z^+) = 0$ with $z^+ \in O_h$ has a unique solution. Now, if $x \in \mathcal{M}_H$ it follows from Proposition 3.9 that $X_H(x)$ is tangential to \mathcal{M} , which means that $dJ(x) \cdot X_H(x) = 0$, so we get $F_0(x) = 0$. Thus, $0 \in F_0(O_0)$, and it follows by smoothness that $0 \in F_h(O_h)$ for small enough h . \square

Remark 4.2. The coisotropy assumption is essential for the result of [Theorem 4.1](#), because it uses [Lemma 3.11](#) which depends on that assumption in an essential manner. On the other hand, if (11) has a unique solution in a neighbourhood of \mathcal{M}^H , then [Assumption 2](#) must hold.

Indeed, the theorem implies that \mathcal{K}_x is locally diffeomorphic to V^* . This implies that their dimension is the same, so $\ker \nu$ must have the same dimension as V^* .

As a result,

$$\dim \ker \nu = \dim V^* = \operatorname{codim} \mathcal{M} = \dim \mathbb{T}\mathcal{M}^\perp.$$

Now, in general $\ker \nu = \mathbb{T}\mathcal{M} \cap \mathbb{T}\mathcal{M}^\perp$, so we get $\mathbb{T}\mathcal{M}^\perp \subset \mathbb{T}\mathcal{M}$, which implies that \mathcal{M} is a coisotropic submanifold.

The result of [Theorem 4.1](#) allows to define the sliding map Γ_{φ_h} by (9). The corresponding SHAKE and RATTLE maps, S_h and R_h , are thus defined when h is sufficiently small.

4.2 Fibre Parametrisation

When the manifold \mathcal{M} is defined implicitly as the locus of functions g_i , one can express the effect of Γ_{φ_h} using the flows of the Hamiltonian vector fields X_{g_i} .

Proposition 4.3. *Suppose that the φ_h -SHAKE method is well defined, so that Γ_{φ_h} is well defined. Under [Assumption 2](#) there exists functions $\lambda_1, \dots, \lambda_m \in \mathcal{C}^\infty(\mathcal{M})$ such that the sliding map Γ_{φ_h} is given by*

$$\Gamma_{\varphi_h}(x) = \exp\left(h \sum_{i=1}^m \lambda_i(x) X_{g_i}\right)(x)$$

Proof. Follows directly from [Corollary 3.7](#). □

4.3 Convergence

We may now show the convergence of SHAKE and RATTLE. The proof is essentially a standard convergence argument for RATTLE, which is a numerical method on the manifold \mathcal{M}^H . The convergence of SHAKE is then obtained using (10).

Proposition 4.4. *Suppose that [Assumption 1](#) and [Assumption 2](#) hold. Let φ_h be a method consistent with $\dot{z} = X_H(z)$. Then the φ_h -SHAKE and φ_h -RATTLE methods are convergent of order at least 1.*

Proof. We first turn to RATTLE. The continuous system is an ordinary differential equation on \mathcal{M}^H with vector field $\mathbb{T}\Pi \circ X_H$ (see [Proposition 3.9](#)). Since it is an ordinary differential equation, we only need to show that RATTLE (defined in [Definition 1.4](#)) is consistent and standard arguments may then be used to show convergence of order 1 (see [7, § II.3]). Using that $R_h = \Pi \circ \varphi_h \circ \Gamma_{\varphi_h}$ and differentiating at $h = 0$ we get

$$\left. \frac{\partial R_h}{\partial h} \right|_{h=0} = \mathbb{T}\Pi \circ \left(\left. \frac{\partial \varphi_h}{\partial h} \right|_{h=0} + \left. \frac{\partial \Gamma_{\varphi_h}}{\partial h} \right|_{h=0} \right),$$

which follows since $\varphi_0 = \operatorname{id}$ and $\Gamma_{\varphi_0} = \operatorname{id}$. The second term is in the kernel of $\mathbb{T}\Pi$, so

$$\left. \frac{\partial R_h}{\partial h} \right|_{h=0} = \mathbb{T}\Pi \circ \left. \frac{\partial \varphi_h}{\partial h} \right|_{h=0}.$$

The assumption that φ_h is consistent with $\dot{z} = X_H(z)$ means that $\left. \frac{\partial \varphi_h}{\partial h} \right|_{h=0} = X_H$. Consistency of R_h then follows.

Now, using (10) and that $\Gamma_{\varphi_h}(z) = z + \mathcal{O}(h)$ when $h \rightarrow 0$, we also get that SHAKE converges of order at least 1. □

Remark 4.5. Interestingly, the local error of SHAKE is only $\mathcal{O}(h)$, so standard arguments do not apply to show convergence. However, due to the fact that SHAKE is the same fibre mapping as RATTLE, this error does not accumulate, and the global error is still $\mathcal{O}(h)$.

4.4 Symplecticity

We examine in which sense SHAKE and RATTLE may be regarded as symplectic method. The essential result is that both SHAKE and RATTLE are *presymplectic*, i.e., they preserve the presymplectic structure of \mathcal{M} .

Proposition 4.6. *Let φ_h be a symplectic method. Then the corresponding SHAKE map S_h and RATTLE map R_h , regarded as mappings $\mathcal{M} \rightarrow \mathcal{M}$, are presymplectic.*

Proof. Since Γ_{φ_h} is trivially presymplectic, it is in particular presymplectic, so

$$\nu(u, v) = \nu(\mathbb{T}\Gamma_{\varphi_h} \cdot u, \mathbb{T}\Gamma_{\varphi_h} \cdot v), \quad \forall u, v \in \mathbb{T}\mathcal{M}.$$

Further, since φ_h is symplectic it follows that

$$\begin{aligned} \nu(u, v) &= \nu(\mathbb{T}\varphi_h \cdot (\mathbb{T}\Gamma_{\varphi_h} \cdot u), \mathbb{T}\varphi_h \cdot (\mathbb{T}\Gamma_{\varphi_h} \cdot v)) \\ &= \nu(\mathbb{T}(\varphi_h \circ \Gamma_{\varphi_h}) \cdot u, \mathbb{T}(\varphi_h \circ \Gamma_{\varphi_h}) \cdot v) \\ &= \nu(\mathbb{T}S_h \cdot u, \mathbb{T}S_h \cdot v), \quad \forall u, v \in \mathbb{T}\mathcal{M}. \end{aligned}$$

Thus, S_h is presymplectic.

Moreover, since $R_h = \Pi \circ S_h$ and Π is trivially presymplectic, R_h is also presymplectic. \square

Proposition 4.7. *Let φ_h be a symplectic method. Under Assumption 1 and Assumption 2, the set $\widetilde{\mathcal{M}}^H$ is a symplectic submanifold of \mathcal{M} , with symplectic form $\widetilde{\omega} = i_{\widetilde{\mathcal{M}}^H}^* \nu$.*

Proof. Under Assumption 1 it follows from Theorem 2.7 that the set (\mathcal{M}^H, ϖ) is a symplectic submanifold of \mathcal{M} . We first show that $\widetilde{\mathcal{M}}^H$ is diffeomorphic to \mathcal{M}^H , and thus also a submanifold of \mathcal{M} , by constructing a diffeomorphism $\mathcal{M}^H \rightarrow \widetilde{\mathcal{M}}^H$. Under Assumption 1 and Assumption 2, the map $\Gamma_{\varphi_h} : \mathcal{M}^H \rightarrow \mathcal{M}$ is well defined. Let $z \in \mathcal{M}^H$. By construction it holds that $\ker(\mathbb{T}_z \Gamma_{\varphi_h}) = \mathbb{T}_z \mathcal{K}_z$. Thus, $\mathbb{T}_z \Gamma_{\varphi_h} : \mathbb{T}_z \mathcal{M}^H \rightarrow \mathbb{T}_{\Gamma_{\varphi_h}(z)} \mathcal{M}$ is injective, so $\Gamma_{\varphi_h} : \mathcal{M}^H \rightarrow \Gamma_{\varphi_h}(\mathcal{M}^H)$ is a diffeomorphism. Next, since $\varphi_h : \mathcal{P} \rightarrow \mathcal{P}$ is a diffeomorphism, it also holds that $\varphi_h : \Gamma_{\varphi_h}(\mathcal{M}^H) \rightarrow \varphi_h(\Gamma_{\varphi_h}(\mathcal{M}^H)) = \widetilde{\mathcal{M}}^H$ is a diffeomorphism. Thus, $S_h = \varphi_h \circ \Gamma_{\varphi_h}$ is a diffeomorphism as a map $\mathcal{M}^H \rightarrow \widetilde{\mathcal{M}}^H$, so \mathcal{M}^H and $\widetilde{\mathcal{M}}^H$ are diffeomorphic.

Next, we show that the form $\widetilde{\omega} = i_{\widetilde{\mathcal{M}}^H}^* \nu$ is nondegenerate. Let $y = S_h(z)$ and $u, v \in \mathbb{T}_y \widetilde{\mathcal{M}}^H$. From Proposition 4.6 it follows that S_h is presymplectic, so

$$\nu(u, v) = \nu(\mathbb{T}_y S_h^{-1} \cdot u, \mathbb{T}_y S_h^{-1} \cdot v) = \varpi(\mathbb{T}_y S_h^{-1} \cdot u, \mathbb{T}_y S_h^{-1} \cdot v).$$

Since $\mathbb{T}_y S_h^{-1} : \widetilde{\mathcal{M}}^H \rightarrow \mathcal{M}^H$ is invertible, and since (\mathcal{M}^H, ϖ) is a symplectic submanifold, it follows that $\nu(u, v) = 0$ for all $v \in \mathbb{T}_y \widetilde{\mathcal{M}}^H$ only if $u = 0$, which shows that $(\widetilde{\mathcal{M}}^H, \widetilde{\omega})$ is a symplectic manifold. \square

The following result follows directly from Theorem 2.7, Proposition 4.6 and Proposition 4.7.

Corollary 4.8. *Let φ_h be a symplectic method and assume that Assumption 1 and Assumption 2 hold. Then:*

- The SHAKE map S_h , regarded a mapping $\widetilde{\mathcal{M}}^H \rightarrow \widetilde{\mathcal{M}}^H$, is symplectic.
- The RATTLE map R_h , regarded as a mapping $\mathcal{M}^H \rightarrow \mathcal{M}^H$, is symplectic.

4.5 Time Reversibility

Just as in the holonomic case, if the underlying method φ_h is *symmetric*, i.e., $\varphi_h^{-1} = \varphi_{-h}$, then RATTLE is also symmetric and thus of second order. Note that SHAKE can never be symmetric, because although S_h preserves $\widetilde{\mathcal{M}}^H$, the reverse method S_{-h} does not.

Proposition 4.9. *If the underlying method φ_h is symmetric, then so is RATTLE, considered as a method from \mathcal{M}^H to \mathcal{M}^H .*

Proof. This follows from the symmetry property of the map Γ_{φ_h} . In general, if $z_0^+ = \Gamma_{\varphi}(z_0)$, $z_1^- = \varphi(z_0^+)$, and $z_1 = \Pi(z_1^-)$ (see Figure 1), then

$$z_1^- = \Gamma_{\varphi^{-1}}(z_1). \quad (13)$$

This follows from Theorem 4.1, because z_1^- is a solution of the equation $J(\varphi^{-1}(z_1)) = 0$, so it must be equal to $\Gamma_{\varphi^{-1}}(z_1)$.

Suppose that we start from a point $z_0 \in \mathcal{M}^H$. The image by the RATTLE map is $z_1 = R_h(z_0)$. Now, since $z_0 = \Pi(z_0^+)$ (as we assumed that $z_0 \in \mathcal{M}^H$), and (13), we obtain $z_0 = \Pi \circ \varphi_h^{-1} \circ \Gamma_{\varphi_h^{-1}}$.

If we assume now that φ_h is symmetric, i.e., $\varphi_h^{-1} = \varphi_{-h}$, we obtain $z_0 = R_{-h}(z_1)$, so RATTLE is symmetric. \square

5 Examples

In this section we give examples of constrained problems that can be solved with the geometric SHAKE and RATTLE methods. In §5.2 we also give non-trivial examples where the nondegeneracy assumption fail to hold.

5.1 Holonomic Case

In this section we study the classical, so-called *holonomic* case, where the constraints depend only on the position q , and not on the momentum p .

Consider the classical case of constrained mechanical systems, where the symplectic manifold \mathcal{P} is simply \mathbf{R}^{2n} , with coordinates (q^i, p_i) , equipped with the canonical symplectic form $\omega = \sum_i dq^i \wedge dp_i$. The constraints are given by $g(q) = 0$ for a function g defined from \mathcal{P} to $V := \mathbf{R}^m$. It should be emphasized that g does not depend on p , i.e., $g_p = 0$. The leaf passing through the point $z = (q, p)$ is then an affine subspace described parametrically by

$$\{ (q, p + g_q(q)^T \lambda) : \lambda \in \mathbf{R}^m \}.$$

Assumption 2 is automatically fulfilled, because $\frac{\partial g_i}{\partial p_j} = 0$ implies

$$\{g_i, g_j\} = 0.$$

Moreover, the standard assumption placed on the Hamiltonian H is that the matrix

$$g_q(q)H_{pp}(q, p)g_q(q)^T \quad \text{be invertible,} \quad (14)$$

(see [8, § VII.1.13], [15]), which implies Assumption 1.

Remark 5.1. The condition (14) is in fact more stringent than Assumption 1, since we only need it at critical points of H on a leaf, i.e., on the points lying on the hidden constraint manifold \mathcal{M}^H . It is clear that the condition (14) is too restrictive when the leaves are compact. We will examine such an example in §5.4.

5.1.1 Classical SHAKE and RATTLE

The classical SHAKE method is only defined for separable Hamiltonian functions (see [8, § VII.1.23], [15], [11]). However, it is readily extended to general Hamiltonian as the mapping $(q_0, p_0) \mapsto (q_1, p_1^-)$ defined by

$$\begin{aligned} p_0^+ &= p_0 - \frac{h}{2} g_q(q_0)^\top \lambda \\ p_{1/2} &= p_0^+ - \frac{h}{2} H_q(q_0, p_{1/2}) \\ q_1 &= q_0 + \frac{h}{2} (H_p(q_0, p_{1/2}) + H_p(q_1, p_{1/2})) \\ p_1^- &= p_{1/2} - \frac{h}{2} H_q(q_1, p_{1/2}) \\ 0 &= g(q_1). \end{aligned}$$

The classical RATTLE method is obtained by adding a projection step onto the manifold \mathcal{M}^H , i.e., the next step is instead $(q_1, p_1^-) \mapsto (q_1, p_1)$ defined, on top of SHAKE, as

$$\begin{aligned} p_1 &= p_1^- + g_q(q_1)^\top \mu \\ 0 &= g_q(q_1) H_p(q_1, p_1). \end{aligned}$$

We see that the mapping $(q_0, p_0^+) \mapsto (q_1, p_1^-)$ is the Störmer-Verlet method, so the classical SHAKE and RATTLE methods are obtained using the Störmer-Verlet method as the underlying unconstrained symplectic method.

Similarly, in [8, § VII.1.3], a first order method is described as

$$\begin{aligned} p_0^+ &= p_0 - h g_q(q_0)^\top \lambda \\ p_1^- &= p_0^+ - h H_q(q_0, p_1^-) \\ q_1 &= q_0 + h H_p(q_0, p_1^-) \\ 0 &= g(q_1) \end{aligned}$$

We see that the mapping $(q_0, p_0^+) \mapsto (q_1, p_1^-)$ is the symplectic Euler method, so this is the SHAKE method obtained using symplectic Euler as the underlying unconstrained symplectic method. When complemented with the projection step

$$\begin{aligned} p_1 &= p_1^- - h g_q(q_1)^\top \mu \\ 0 &= g_q(q_1) H_p(q_1, p_1), \end{aligned}$$

that method becomes the corresponding RATTLE method.

5.2 Examples of Failing Nondegeneracy Assumption

Let us examine an example where [Assumption 1](#) is not fulfilled. The manifold \mathcal{P} is \mathbf{R}^4 with coordinates q, p, \bar{q}, \bar{p} , and the symplectic form is $\omega = dq \wedge dp + d\bar{q} \wedge d\bar{p}$. The constraint function J is

$$J(q, p, \bar{q}, \bar{p}) = \bar{q}.$$

The corresponding leaves are the lines parametrised by \bar{p} , i.e., the leaves are the lines of equation $(q, p, \bar{q}) = (q_0, p_0, \bar{q}_0)$. We choose the Hamiltonian

$$H = \frac{p^2}{2} + \bar{p}q.$$

The hidden constraint manifold is then $\mathcal{M}^H = \{q = 0\}$. The restriction of H on a leaf is a linear function (because H is linear in \bar{p}), so its critical points are degenerate, and [Assumption 1](#) is not fulfilled. As a result, there are extra constraints which prevent the problem from being well-posed on \mathcal{M}^H . It is readily verified that the system has in fact index five instead of three, the tertiary and quaternary constraints being respectively $p = 0$ and $\bar{p} = 0$.

If we had assumed instead that $H = \frac{p^2}{2}$, the hidden constraint set would be $\mathcal{M}^H = \mathcal{M}$, because H is now constant on the leaves (because H does not depend on \bar{p}). In that case, there are infinitely many solutions to the problem at hand.

5.3 Index 1 Constraints

Let $\mathcal{P} = \mathbf{R}^{2n+2k}$ with coordinates $q \in \mathbf{R}^n$, $p \in \mathbf{R}^n$, $\alpha \in \mathbf{R}^k$, $\beta \in \mathbf{R}^k$, symplectic form $\omega = dq \wedge dp + d\alpha \wedge d\beta$, Hamiltonian $H(q, p, \beta)$, and consider the holonomic constraint $\alpha = 0$. Because the constraints are holonomic, the coisotropy assumption is satisfied (see [§ 5.1](#)). The presymplectic manifold is $\mathcal{M} = \mathbf{R}^{2n+k}$ with coordinates (q, p, β) and presymplectic form $\nu = dq \wedge dp$. The hidden constraint submanifold is $\mathcal{M}^H = \{(q, p, \lambda) : H_\beta(q, p, \beta) = 0\}$, giving the presymplectic system

$$\begin{aligned} \dot{q} &= H_p(q, p, \beta) \\ \dot{p} &= -H_q(q, p, \beta) \\ 0 &= H_\beta(q, p, \beta) \end{aligned} \tag{15}$$

The nondegeneracy assumption is that $H_{\beta\beta}$ is nonsingular on \mathcal{M}^H . When this holds, the secondary constraint can be solved for $\beta = B(q, p)$. This is the case of index one constraints considered in [\[14\]](#). In this paper, a symplectic integrator is introduced and studied for the index one constrained Hamiltonian system [\(15\)](#), consisting of a direct application of a symplectic Runge–Kutta method to the full system [\(15\)](#). In the case when φ_h is the midpoint rule, we now show that this method is equivalent to the application of SHAKE or RATTLE applied on \mathcal{P} . Indeed, Hamilton's equations on \mathcal{P} are given by

$$\begin{aligned} \dot{q} &= H_p(q, p, \beta) \\ \dot{p} &= -H_q(q, p, \beta) \\ \dot{\alpha} &= H_\beta(q, p, \beta) \\ \dot{\beta} &= 0 \end{aligned}$$

for which the midpoint discretization, defining φ_h , is

$$\begin{aligned} \frac{q_1 - q_0}{h} &= H_p\left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}, \frac{\beta_0 + \beta_1}{2}\right) \\ \frac{p_1 - p_0}{h} &= -H_q\left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}, \frac{\beta_0 + \beta_1}{2}\right) \\ \frac{\alpha_1 - \alpha_0}{h} &= H_\beta\left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}, \frac{\beta_0 + \beta_1}{2}\right) \\ \beta_1 - \beta_0 &= 0 \end{aligned} \tag{16}$$

while the constraint flow is given by $\exp(\lambda^T X_\alpha) : (q, p, \alpha, \beta) \mapsto (q, p, \alpha, \beta - \lambda)$. Initially, the primary constraints are satisfied, i.e. $\alpha_0 = 0$, and the constraint flow determines β_1 so that $\alpha_1 = 0$, i.e., so that

$$0 = H_\beta\left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}, \frac{\beta_0 + \beta_1}{2}\right)$$

with solution $\frac{\beta_0 + \beta_1}{2} = B\left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}\right)$. This is exactly the method of [14] in the case of the midpoint rule. The final step of RATTLE chooses β so that $0 = H_\beta(q_1, p_1, \beta)$, but (as we have seen in the general case), this value is irrelevant for the next step.

5.4 Harmonic Constraints

Consider the symplectic manifold \mathcal{P} defined by

$$\mathcal{P} := \mathbf{C}^2 \simeq \mathbb{T}^*\mathbf{R}^2, \quad (17)$$

with coordinates

$$z_0 = q_0 + ip_0, \quad z_1 = q_1 + ip_1,$$

and the canonical symplectic form

$$\omega(q_0, p_0, q_1, p_1) = dq_0 \wedge dp_0 + dq_1 \wedge dp_1.$$

We will sometimes use the notation $\mathbf{q} = (q_0, q_1)$ and $\mathbf{p} = (p_0, p_1)$.

The constraint space is $V = \mathbf{R}$, and the single constraint function is

$$g(\mathbf{q}, \mathbf{p}) := \|\mathbf{q}\|^2 + \|\mathbf{p}\|^2 - 1.$$

Note that the corresponding manifold \mathcal{M} is S^3 , i.e., the unit sphere in \mathbf{R}^4 . It is automatically a coisotropic submanifold since it has codimension one (see Remark 3.4). The foliation induced by g is the Hopf fibration of the 3-sphere in circles. The Hopf map

$$(z_0, z_1) \mapsto (2z_0\bar{z}_1, |z_0|^2 - |z_1|^2) \quad (18)$$

projects \mathbf{C}^2 onto $\mathbf{R}^3 \equiv \mathbf{C} \times \mathbf{R}$ and maps 3-sphere onto 2-spheres. The quotient manifold $\overline{\mathcal{M}}$ is thus diffeomorphic to a 2-sphere.

The flow of the Hamiltonian vector field X_g is

$$\exp(X_g t)(z_0, z_1) = (e^{it}z_0, e^{it}z_1). \quad (19)$$

5.4.1 Hamiltonian without Potential Energy

In this section, we examine the validity of Assumption 1 for the simple Hamiltonian function given by

$$H(\mathbf{q}, \mathbf{p}) = \frac{\|\mathbf{p}\|^2}{2}.$$

The equations (5) are in this case

$$\begin{aligned} \dot{\mathbf{q}} &= (1 + \lambda)\mathbf{p} \\ \dot{\mathbf{p}} &= -\lambda\mathbf{q} \\ 1 &= \|\mathbf{q}\|^2 + \|\mathbf{p}\|^2. \end{aligned} \quad (20)$$

Let us look at the restriction \mathcal{H} of H on a leaf parametrized by $\theta \in \mathbf{R}/\mathbf{Z}$, passing by the point (\mathbf{q}, \mathbf{p}) for $\theta = 0$. We obtain after trigonometric simplification

$$\mathcal{H}(\theta) = \frac{1}{4} \left(\|\mathbf{p}\|^2 (1 + \cos(2\theta)) + \|\mathbf{q}\|^2 (1 - \cos(2\theta)) + 2\mathbf{q} \cdot \mathbf{p} \sin(2\theta) \right).$$

One checks that $\mathcal{H}(0) = H(\mathbf{q}, \mathbf{p}) = \|\mathbf{p}\|^2/2$. By differentiating, one obtains

$$\mathcal{H}'(\theta) = \frac{1}{2} \left((\|\mathbf{q}\|^2 - \|\mathbf{p}\|^2) \sin(2\theta) + 2\mathbf{q} \cdot \mathbf{p} \cos(2\theta) \right). \quad (21)$$

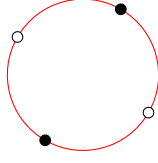


Figure 2: An illustration of the intersection of a leaf with \mathcal{M}^H . The two opposite points on each leaf are part of the same connected component of \mathcal{M}^H .

We know that the point (\mathbf{q}, \mathbf{p}) lies in \mathcal{M}^H if $\mathcal{H}'(0) = 0$, which leads to

$$\mathcal{M}^H = \{ (q_0, p_0, q_1, p_1) \in \mathcal{M} : \mathbf{q} \cdot \mathbf{p} = 0 \}. \quad (22)$$

This could also have been derived by differentiating the constraints in the differential algebraic equation (20), or by using one of the equivalent formulations of Remark 3.10.

Such a point is a nondegenerate critical point for \mathcal{H} if and only if $\|\mathbf{q}\|^2 - \|\mathbf{p}\|^2 \neq 0$. We also see that if (\mathbf{q}, \mathbf{p}) is a degenerate critical point, then $\mathbf{q} \cdot \mathbf{p} = 0$ and $\|\mathbf{q}\| = \|\mathbf{p}\|$, so H is constant on the whole leaf. A closer examination shows that there are two such leaves, which are mapped to the 2-sphere to the antipodal points $(i, 0)$ and $(-i, 0)$ by the Hopf map. We call those two points the *exceptional points*.

Let us turn to the intersection of \mathcal{M}^H on each leaf. The form of (21) shows that \mathcal{H} has four distinct critical points on each leaf. Moreover, two such points are such that $\|\mathbf{q}\| > \|\mathbf{p}\|$ where as the two others are such that the opposite inequality holds. The points are intertwined, see Figure 2. Interestingly, it is possible to join two opposite points on the fibre by a homotopy curve of the following form. If $\|\mathbf{q}\| < \|\mathbf{p}\|$, then we choose the homotopy

$$[-1, 1] \ni t \mapsto (t\mathbf{q}, \mathbf{p}),$$

whereas if $\|\mathbf{p}\| < \|\mathbf{q}\|$, we choose the obvious other homotopy, where \mathbf{p} and \mathbf{q} are swapped. This shows that if one removes the leaves above the two exceptional points, the set \mathcal{M}^H is a manifold with two connected components.

Note that $\|\mathbf{q}\|$ and $\|\mathbf{p}\|$ are constant on each trajectory, so the trajectories never meet the exceptional points.

Let us gather our findings:

Proposition 5.2. *Consider the symplectic manifold \mathcal{P} defined by (17), and the constraint submanifold defined by*

$$\mathcal{M} := \left\{ (z_0, z_1) \in \mathcal{P} : |z_0|^2 + |z_1|^2 = 1 \quad \text{and} \quad (2z_0\bar{z}_1, |z_0|^2 - |z_1|^2) \neq (\pm i, 0) \right\}.$$

Then both Assumption 1 and Assumption 2 hold. The hidden constraint manifold \mathcal{M}^H is defined by (22). It has two connected components. Each of those components crosses each leaf of \mathcal{K} twice, as depicted on Figure 2. Moreover, the vector field defined on \mathcal{M}^H is complete, i.e., all the trajectories exist for all time.

5.4.2 Hamiltonian with Linear Potential Energy

We now choose the Hamiltonian

$$H = \frac{\|\mathbf{p}\|^2}{2} - \mathbf{g} \cdot \mathbf{q} \quad (23)$$

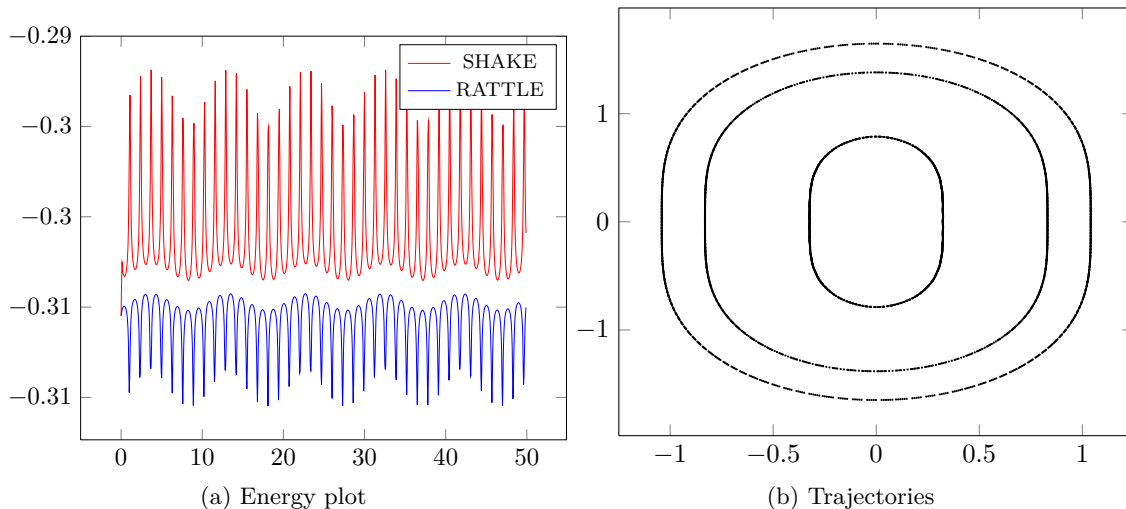


Figure 3: Some simulation results for the Hamiltonian (23) with the vector $\mathbf{g} := (0, -1)$. Both the SHAKE and RATTLE methods use the midpoint rule as underlying unconstrained symplectic integrator. The time step is $h = 0.1$ in all the examples. We choose the initial conditions in Table 1. The plot (a) shows an energy plot for the SHAKE and RATTLE methods for the initial condition z_0 . The plot (b) shows the three trajectories for the initial conditions z_0, z_1 and z_2 . We first use the Hopf map described in (18) and then use a stereographic projection.

z_0	z_1	z_3
-0.7865261200000000	-0.4963624948824013	0.3477491188213400
-0.4043988000000000	-0.7319740436366664	-0.8131619010029159
-0.3880746864163783	-0.4275775933953260	-0.4368285559113795
0.2173391755798215	0.1225384882604160	-0.0837800227934176
-1.3703247300000001	-1.3703247300000001	-1.3703247300000001

Table 1: Three initial conditions used in Figure 3. The fifth component is the Lagrange multiplier.

where \mathbf{g} is a fixed given vector.

Now the structure of the hidden constraint manifold \mathcal{M}^H is more involved. In particular, there are many singular points where the set \mathcal{M}^H ceases to be a manifold. For that reason it is somewhat difficult to find entire trajectories which stay on the patches of \mathcal{M}^H which are manifolds. We nevertheless present in Figure 3 simulated trajectories for initial conditions such that those trajectories do not meet any singular point.

6 Discussion

The geometric version of the Dirac constraint algorithm [4] in the instance used here delivers a chain of submanifolds

$$\mathcal{M}^H \hookrightarrow \mathcal{M} \hookrightarrow \mathcal{P}$$

in which \mathcal{M}^H is symplectic. The geometric RATTLE algorithm delivers symplectic integrators on \mathcal{M}^H . However, \mathcal{P} , the intervening presymplectic manifold \mathcal{M} , its coisotropy,

and knowledge of its fibers, are essential to the algorithm. If the fibers cannot be explicitly parametrized, the algorithm is still formally defined, but more computation would be required in practice—for example, by integrating the fibers numerically to roundoff error. This is an extreme version of a situation common in numerical analysis, in which allowing a wider class of methods (e.g. implicit Runge–Kutta methods, for which implicit equations have to be solved numerically) enables a wider class of properties.

If \mathcal{M} is not coisotropic, then the coisotropic embedding theorem [5] says that there exists a symplectic manifold \mathcal{P}' such that \mathcal{M} is coisotropically embedded in \mathcal{P}' (Remark 3.3). Thus, abstractly at least, one can extend the Hamiltonian on \mathcal{M} arbitrarily to \mathcal{P}' and apply the geometric RATTLE algorithm, for the rest of the required structure is intrinsic to \mathcal{M} . In specific examples it may be possible to carry this out by finding a suitable symplectic vector space \mathcal{P}' . The same remark holds if the given data is a Hamiltonian on a presymplectic manifold, see §5.3.

However there remain many constrained problems which do not fall into the classes considered here. The most fundamental one has data $(\mathcal{P}, \mathcal{M}', H)$ where \mathcal{M}' is a symplectic submanifold of the symplectic manifold \mathcal{P} . We do not know of symplectic integrators for this problem. They would provide symplectic integrators for a wide class of symplectic manifolds. A very general situation is that provided by the geometric version of the Dirac constraint algorithm [4], which, from presymplectic data (\mathcal{M}, ω, H) , produces a nested sequence of submanifolds

$$\mathcal{M}_K \hookrightarrow \mathcal{M}_{K-1} \hookrightarrow \dots \hookrightarrow \mathcal{M}_1 := \mathcal{M}$$

defined by

$$\mathcal{M}_{K+1} := \{x \in \mathcal{M}_K : dH(x) \in \omega(\mathcal{M}_K)\}$$

and a (possibly nonunique) vector field X such that $\iota_{\mathcal{M}_K}(i_X\omega - dH) = 0$. One would like to integrate an index- K DAE on \mathcal{M} or an index- $K + 1$ DAE on a symplectic embedding of \mathcal{M} so as to preserve the constraints and $\iota_{\mathcal{M}_K}\omega$.

Finally, we mention another class of integrators for the holonomic case, known as SPARK, for Symplectic Partitioned Additive Runge–Kutta [9]. These generalise RATTLE to higher order. They are *partitioned* (use different RK coefficients for the q and p components) and *additive* (use different RK coefficients for the constraint and regular forces). The holonomic assumption is used in two critical steps: first, it means that the flow of the constraint force is given by Euler’s method; second, it means that the q -component of the constraint forces vanishes. This allows their RK coefficients to be arbitrary, which means that the RK coefficients of the p -component can be arbitrary, and can be chosen to include stages at the endpoints. Thus, this approach does not immediately give an algorithm for problems of the type $(\mathcal{P}, \mathcal{M}', H)$ mentioned above. The situation is similar to the relationship between splitting methods and RK methods; we do not know if SPARK can be adapted to more general constraints.

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References

- [1] H. C. Andersen. Rattle: A “velocity” version of the shake algorithm for molecular dynamics calculations. *Journal of Computational Physics*, 52(1):24 – 34, 1983. ISSN 0021-9991. doi: 10.1016/0021-9991(83)90014-1. URL <http://www.sciencedirect.com/science/article/pii/0021999183900141>. 4
- [2] P. Dirac. *Lectures on quantum mechanics*. Dover Books on Physics Series. Dover Publications, 2001. ISBN 9780486417134. 5
- [3] Z. Ge and J. E. Marsden. Lie-Poisson Hamilton-Jacobi theory and Lie-Poisson integrators. *Phys. Lett. A*, 133(3):134–139, 1988. doi: 10.1016/0375-9601(88)90773-6. 7
- [4] M. Gotay, J. Nester, and G. Hinds. Presymplectic manifolds and the dirac–bergmann theory of constraints. *Journal of Mathematical Physics*, 19:2388, 1978. doi: 10.1063/1.523597. 5, 24, 25
- [5] M. J. Gotay. On coisotropic imbeddings of presymplectic manifolds. *Proc. Am. Math. Soc.*, 84(1):111–114, 1982. doi: 10.2307/2043821. 12, 25
- [6] V. Guillemin and S. Sternberg. *Symplectic techniques in physics*. Cambridge University Press, 1990. ISBN 9780521389907. 7
- [7] E. Hairer, S. Nørsett, and G. Wanner. *Solving ordinary differential equations: Non-stiff problems*. Springer series in computational mathematics. Springer, 1993. ISBN 9783540566700. 17
- [8] E. Hairer, C. Lubich, and G. Wanner. *Geometric numerical integration: structure-preserving algorithms for ordinary differential equations*. Springer series in computational mathematics. Springer, 2006. ISBN 9783540306634. 4, 19, 20
- [9] L. Jay. Symplectic partitioned Runge-Kutta methods for constrained Hamiltonian systems. *SIAM J. Numer. Anal.*, 33(1):368–387, 1996. ISSN 0036-1429. doi: 10.1137/0733019. URL <http://dx.doi.org/10.1137/0733019>. 4, 25
- [10] B. Leimkuhler and S. Reich. *Simulating Hamiltonian Dynamics*, volume 14 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge University Press, Cambridge, 2004. ISBN 9780521772907. 4
- [11] B. Leimkuhler and R. Skeel. Symplectic numerical integrators in constrained hamiltonian systems. *Journal of Computational Physics*, 112(1):117–125, 1994. doi: 10.1006/jcph.1994.1085. 4, 20
- [12] P. Libermann and C. Marle. *Symplectic geometry and analytical mechanics*. Mathematics and its applications. D. Reidel, 1987. ISBN 9789027724380. 7
- [13] J. Marsden and T. Ratiu. *Introduction to mechanics and symmetry: a basic exposition of classical mechanical systems*. Texts in applied mathematics. Springer, 1999. ISBN 9780387986432. 4
- [14] R. McLachlan, K. Modin, O. Verdier, and M. Wilkins. Symplectic integrators for index one constraints, 2012. In preparation. 21, 22

- [15] S. Reich. Symplectic integration of constrained hamiltonian systems by composition methods. *SIAM journal on numerical analysis*, 33(2):475–491, 1996. doi: 10.1137/0733025. 4, 19, 20
- [16] J.-P. Ryckaert, G. Ciccotti, and H. J. Berendsen. Numerical integration of the cartesian equations of motion of a system with constraints: molecular dynamics of n-alkanes. *Journal of Computational Physics*, 23(3):327 – 341, 1977. ISSN 0021-9991. doi: 10.1016/0021-9991(77)90098-5. URL <http://www.sciencedirect.com/science/article/pii/0021999177900985>. 4