A Symplectic Integrator for Molecular Dynamics on a Hypersphere

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We present a reversible and symplectic algorithm called ROLL, for integrating the equations of motion in molecular dynamics simulations of simple fluids on a hypersphere $S^d$ of arbitrary dimension $d$. It is derived in the framework of Geometric Algebra and shown to be mathematically equivalent to algorithm RATTLE. An application to molecular dynamics simulation of the one component plasma is briefly discussed.

Keywords: Symplectic integrator; Hypersphere; Molecular Dynamics

I. INTRODUCTION

The idea of using the two dimensional (2D) surface of an ordinary sphere, i.e. space $S^2$, to perform Monte Carlo (MC) and/or molecular dynamics (MD) simulations of a 2D fluid can be tracked back to a paper by J.-P. Hansen et al. devoted to a study of the electron gas at the surface of liquid Helium [1]. The generalization to MC simulations of 3D systems, implying the use of a hypersphere as the simulation cell, i.e. the vector manifold $S^3$, is due to Caillol and Levesque [2] in their study of 3D ionic liquids.

Recently, a symplectic integrator for MD simulations of 2D systems on 2-spheres was proposed in references [3, 4]. In this article we extend this integrator to 3D systems. This can be done elegantly in the framework of Geometric Algebra (GA) [5–10].

The paper is organized as follows. In section II we discuss the extension of the laws of classical mechanics in an euclidean space of arbitrary dimension $d$, with an emphasis on the correct definition of the angular momentum. In section III we consider the motion of classical point particles confined on the surface of a hypersphere from the point of view of GA formalism. GA is briefly described in appendix A. We derive the algorithm ROLL in section IV. ROLL is shown to be equivalent to algorithm RATTLE [11] in appendix B from which it inherits all his properties (reversibility and symplecticity). We then present an application of ROLL to MD simulations of the one component plasma (OCP) in section V. We conclude in section VI.

II. CLASSICAL MECHANICS IN AN EUCLIDEAN SPACE OF ARBITRARY DIMENSION

A. General discussion

Let us first fix some definitions and notations. We associate to the usual inner product space $\mathbb{R}^d$ the euclidean affine space $E^d$, defined as a set of points $M$ such that, given an origin $O$, there is a unique vector $q \in \mathbb{R}^d$ such that $\overrightarrow{OM} = q$. Once $O$ is fixed, we identify the two spaces $E^d$ and $\mathbb{R}^d$. We denote by $\{e_i\}, i = 1 \ldots n$, the standard orthonormal basis of $E^d$ with the property that $e_i \cdot e_j = \delta_{ij}$, where $\cdot$ is the usual scalar product of $\mathbb{R}^d$ and $\delta_{ij}$ the Kronecker symbol.

Extending the laws of classical mechanics to a space $E^d$ of arbitrary dimension $d > 3$ causes no problem, except for those quantities or laws involving, as the angular momentum for instance, the cross product of two vectors $a$ and $b$. In physical space $E^3$, the cross product $a \times b$ is an axial vector, perpendicular to the 2-plane span($a, b$) and of a magnitude equal to the area of the parallelogram with edges $a$ and $b$ (cf the definition (A2) in appendix A). The point is that this definition of the outer product $a \times b$ can be extended to an algebra $G^d$ of arbitrary dimension $d$, contrary to the cross product defined only for $d = 3$.

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So, for a system of $N$ point particles (positions $q_\alpha$, linear momenta $p_\alpha = m_\alpha \dot{q}_\alpha$ (as usual dots denote time derivative), $\alpha = 1 \ldots N$) of $E^d$, we are led to define the angular momentum as \[ K = \sum_{\alpha=1}^{N} q_\alpha \wedge p_\alpha. \] (1)

$K$ is a bivector of the GA algebra $\mathbb{G}^d$. In dimension $d = 3$ the dual of $K$ is the usual 1-vector angular momentum.

\[ K^* = \sum_{\alpha=1}^{N} q_\alpha \times p_\alpha \ (\text{only for } d = 3). \] (2)

It follows from $\dot{q}_\alpha \wedge p_\alpha = 0$ that a well known theorem of classical mechanics [6, 10, 12] is generalized to arbitrary dimension :

\[ \frac{d}{dt} K = \sum_{\alpha=1}^{N} q_\alpha \wedge f_\alpha, \] (3)

where $f_\alpha$ is the total force acting on particle $\alpha$. Following Goldstein [12] we decompose $f_\alpha$ as the sum of an external force $f^e_\alpha$ and the sum of the pair-wise additive forces due to the other particles $\sum_{\beta \neq \alpha} f_{\beta \alpha}$. If Newton’s weak law of action and reaction holds, i.e. if $f_{\beta \alpha} = -f_{\alpha \beta}$ then we have

\[ \frac{d}{dt} K = \sum_{\alpha=1}^{N} q_\alpha \wedge f^e_\alpha. \] (4)

In the case where there are no external forces, the angular momentum bivector $K$ is a conserved dynamical variable of the motion. This means the conservation of its $(d^2)$ scalar components. As well known, this is a consequence of the rotational invariance of the system, as expressed by Noether’s theorem [10, 12]. As a warm up, let us derive this theorem in the framework of the GA formalism.

### B. Rotational invariance and the conservation of the angular momentum bivector

Henceforth in this section, we restrict ourselves to systems made of $N$ classical point particles with identical masses $m$ living in Euclidean space $E^d$. The Lagrangian reads :

\[ \mathcal{L} (q_\alpha, \dot{q}_\alpha) = \frac{m}{2} \sum_{\alpha=1}^{N} \dot{q}_\alpha^2 - \frac{1}{2} \sum_{\alpha \neq \beta} v(|q_\alpha - q_\beta|), \] (5)

where the pair potential depends only on the distance $|q_\alpha - q_\beta|$ between the particles. Extending Euler-Lagrange equations to an arbitrary dimension $d$ causes no trouble, with the well known result [12]

\[ \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_\alpha} = \frac{\partial \mathcal{L}}{\partial q_\alpha} \text{ for } \alpha = 1 \ldots N. \] (6)

We apply now Noether theorem to the Lagrangian function [13]. Clearly $\mathcal{L} (q_\alpha, \dot{q}_\alpha)$ is invariant under any rotation of $O(d)$ of center $O$. An elemental rotation of space $E^d$ is described firstly by its invariant plane, containing the origin, and represented by some unit bivector $i$ (with $i^2 = -1$), and secondly, by a (scalar) magnitude $\theta$. Bivector $\Omega = i\theta$ is called the angle of the rotation. The action of this rotation is described by a member of the geometric algebra $\mathbb{G}^d$, $R$, called a rotor (or a generalized complex number) defined as [8–10, 13]

\[ R = \exp \left( -\frac{\Omega}{2} \right) = \cos \frac{\theta}{2} - \sin \frac{\theta}{2} i. \] (7)

Under the rotation every element $A$ of the algebra is transformed according to the law

\[ A = RAR^{-1}, \] (8)
where the inverse of $R$, $R^{-1} = R^\dagger = \exp(+\Omega/2)$. Therefore, for an infinitesimal rotation $\delta\Omega$, the variation of $q_\alpha$ is given by

$$ \delta q_\alpha = \frac{1}{2} (q_\alpha \delta\Omega - \delta\Omega q_\alpha) + O((\delta\Omega)^2)_1 $$

$$ = q_\alpha \cdot \delta\Omega + O((\delta\Omega)^2)_1 $$

(9)

where the medium-dot "," denotes the inner product of the algebra, cf equation (A3a). idem, the variations of the velocities are given by

$$ \delta \dot{q}_\alpha = \dot{q}_\alpha \cdot \delta\Omega + O((\delta\Omega)^2)_1 $$

(10)

The infinitesimal rotation yields the following variation for the lagrangian

$$ \delta \mathcal{L} = \sum_{\alpha=1}^{N} \left( \frac{\partial \mathcal{L}}{\partial q_\alpha} \cdot (q_\alpha \cdot \delta\Omega) + \frac{\partial \mathcal{L}}{\partial \dot{q}_\alpha} \cdot (\dot{q}_\alpha \cdot \delta\Omega) \right) , $$

(11)

where we took care of the non-associativity of the inner product. However, by taking into account Euler-Lagrange equations as well as the identity (A8) of appendix A, equation (11) can be recast as

$$ \delta \mathcal{L} = \left( \frac{d}{dt} \sum_{\alpha=1}^{N} p_\alpha \wedge q_\alpha \right) \cdot \delta\Omega , $$

(12)

were we introduced momentum $p_\alpha = \partial \mathcal{L}/\partial \dot{q}_\alpha = m\dot{q}_\alpha$. Requiring that $\delta \mathcal{L} = 0$ for any arbitrary infinitesimal bivector $\delta\Omega$ yields, as expected, the conservation of the total angular momentum $K$ :

$$ \frac{d}{dt} \sum_{\alpha=1}^{N} q_\alpha \wedge p_\alpha = 0 . $$

(13)

### III. CLASSICAL MECHANICS ON A HYPERSPHERE

#### A. The bivector angular velocity

The hypersphere $S^d(O,R)$ of center $O$ and radius $R$, i.e. the set of points $M$ of $E^{d+1}$ such that $\overrightarrow{OM}^2 = q^2 = R^2$, may be seen as a $d$-dimensional vector manifold of the euclidean space $E^{d+1}$ [7]. It is convenient to introduce the unit hypersphere $S^d = S^d(O,R = 1)$ of unit vectors $\xi = q/R$. The space $E^d_\xi$ tangent to $S^d(O,R)$ at point $q = R\xi$ plays a central role, here live the particle velocities. It is an euclidean hyperplane of dimension $d$, spanned by the $d$ orthonormal vectors $\{e_i(\xi)\}$, $i = 1, \ldots, d$. When complemented with vector $\xi$, this system of vectors forms a local orthonormal basis of full space $E^{d+1}$. $E^d_\xi$ is represented by its unit pseudo-scalar $I^d(\xi) = e_1(\xi)e_2(\xi) \ldots e_n(\xi)$ [7, 10]. Vector $\xi$ and the d-blade $I^d(\xi)$ are related by a duality relation [A6], hence $\xi^* = \pm I^d(\xi)$, the sign depending of the orientation of the local basis of $E^{d+1}$. Therefore, the projection of any blade $A$ of $\mathbb{G}^{d+1}$ onto $E^d_\xi$ is given by $\text{A77}$

$$ P_{\xi^*}(A) = ( A \cdot \xi^* ) (\xi^*)^{-1} , $$

(14)

which gives, in the case of a vector $a \in E^{d+1}$

$$ P_{\xi^*}(a) = a - (\xi, a) \xi . $$

(15)

Let us consider the dynamics of a single point particle $q$ on $S^d(O,R)$. Its dynamics is that of a rotator of $E^{d+1}$ : its position at time $t$ can be obtained from that at time $t = 0$ by a rotation of $O(d+1)$ of center $O$ described by some rotor $R(t)$. We thus have [6, 10]

$$ \xi(t) = R(t)\xi_0 R^\dagger(t) , $$

(16)

where $R^\dagger(t) = R^{-1}(t)$ is the reverse of $R(t)$ [6, 7, 10]. Taking the time derivative of equation (16) one finds that

$$ \dot{\xi} = \xi \cdot \Omega , $$

(17)
where the angular velocity $\Omega(t)$ is a bivector defined by

$$\Omega = -2\dot{R}R^\dagger.$$  \hfill (18)

At this point it must be stressed that equation (16) does not fully determine the rotor $R(t)$ (and thus $\Omega(t)$). Recall that an elemental rotation of $O(d + 1)$ is defined by a 2-plane and an amplitude. If this plane is a subspace of the tangent hyperplane $\xi^*$ then it lets vector $\xi$ unchanged. Therefore there is some freedom and, in order to fix it, we decompose $\Omega$ upon the standard basis of the bivectors of the algebra

$$\Omega = \Omega^\perp + \Omega^\parallel$$  \hfill (19a)

$$\Omega^\perp = P_{\xi^*}(\Omega) = \sum_{1 \leq \alpha < \beta \leq d} \Omega^\perp_{\alpha\beta} e_\alpha(\xi) \wedge e_\beta(\xi)$$  \hfill (19b)

$$\Omega^\parallel = \sum_{1 \leq \alpha \leq d} \Omega^\parallel_\alpha e_\alpha(\xi) \wedge \xi.$$  \hfill (19c)

One readily obtains from expansion (19b) that $\xi \cdot \Omega^\perp = \langle \xi \Omega^\perp \rangle_1 = 0$ and thus $\xi \cdot \Omega = \xi \cdot \Omega^\parallel$. Similarly, from (19c) one deduces that $\xi \wedge \Omega^\parallel = 0$ and thus $\xi \wedge \Omega = \xi \wedge \Omega^\perp$. It is thus possible to chose $\Omega^\perp = 0$ which fully determines the angular velocity. It amounts to impose the condition

$$\xi \wedge \Omega = 0.$$  \hfill (20)

Indeed, from $\Omega^\perp = 0$ and $\dot{\xi} = \xi \cdot \Omega$ one obtains all the coefficients of the expansions (19b) and (19c) : $\Omega^\perp_{\alpha\beta} = 0$ and $\Omega^\parallel_\alpha = -\dot{\xi} \cdot e_\alpha(\xi)$, which means that $\Omega = \xi \wedge \dot{\xi} = \dot{\xi} \cdot \xi$. This expression for $\Omega$ shows that the two additional conditions $\xi \wedge \Omega = 0$ and $\xi \wedge \Omega = 0$ also hold.

It is interesting to consider more closely the case $d = 2$ for a comparison with the work of Lee et al. [3]. In this case the dual of bivector $\Omega$ is an axial vector $\omega$ and one recovers the usual expression for the vector angular velocity $\omega = \Omega^* = \xi \times \dot{\xi}$ and the usual relation $\dot{\xi} = \omega \times \xi$ [3]. The condition $\xi \wedge \Omega = 0$ becomes $\xi \cdot \omega = 0$.

### B. Equation of motion on a hypersphere

To simplify the notations we consider the case of a single point particle. For the matters discussed here, the extension to the case of $N$ particles is trivial. This particle, of mass $m$, position $q$, is subjected to some external, unspecified force $f$ and constrained to move on the surface of the sphere $S^d(O, R)$. Again $\xi = q/R$ denotes its position on the unit hypersphere $S^d$.

Two points of view can be adopted : the motion can be either described as a motion in $E^{d+1}$ with holonomic constraints or by the theorem (3) derived in section III A and rederived in section III B 2 using a lagrangian formalism in the framework of GA.

#### 1. Constraints

The mechanical situation is described by the holonomic constraint

$$\sigma(q) = q^2 - R^2 = 0.$$  \hfill (21)

If $f = -\nabla_q V(q)$ the Newton’s equation of motion can be obtained as the Euler-Lagrange equation associated to the constrained Lagrangian $L^* = m\dot{q}^2/2 - V(q) - \lambda \sigma(q)$, it reads [12, 14]

$$m\ddot{q} = f - 2\lambda q.$$  \hfill (22)

The force due to the constraint is thus $-\lambda \nabla_q \sigma = -2\lambda q$, it is of course perpendicular to the tangent plane $\xi^*$. Equation (22) can be simplified as

$$m\ddot{\xi} = \frac{f^\perp}{R} - 2\overline{\lambda} \xi,$$  \hfill (23a)

$$\overline{\lambda} = \lambda - \frac{f \cdot \xi}{2R}.$$  \hfill (23b)
where $f^\perp$ is the projection of the force $f$ in the tangent hyperplane $E^i_q$ (cf equation (24)):

$$f^\perp = P_{\xi^*}(f) = f - (f \cdot \xi)\xi.$$  

(24)

By passing we note that, taking the scalar product of both sides of (23a) with $\xi$ yields $\Xi = (m/2)\dot{\xi}^2$ where we used the "hidden constraint" $\dot{\xi} \cdot \dot{\xi} + \dot{\xi}^2 = 0$ obtained by taking twice the time derivative of the constraint equation (21) valid for all times. $\Xi$ has been eliminated and the equation of motion reads as

$$m\ddot{\xi} = \frac{f^\perp}{R} - m\dot{\xi}\dot{\xi}.$$  

(25)

2. Euler-Lagrange equations

We consider a particle confined on $S^d(0, R)$ with lagrangian $L(q, \dot{q}) = (m/2)\dot{q}^2 - V(q)$ where $V(q)$ is an arbitrary potential. Euler-Lagrange equations are obtained by minimizing the action

$$S = \int_0^T L(q, \dot{q}) \, dt,$$  

(26)

with respect to infinitesimal variations $\delta q(t)$ such that $\delta q(0) = \delta q(T) = 0$. As noted in reference [3] the expression of $\delta q(t)$ must agree with the geometric structure of the configuration manifold, which is not a linear vector space but a group. Referring to our discussion of section III A we are led to consider $\delta q = q \cdot \delta \Theta$ where $\delta \Theta(t)$ is, as the angular velocity $\Omega(t)$, an arbitrary infinitesimal time-dependent bivector subject to the condition $q \wedge \delta \Theta = 0$, i.e. $\delta \Theta_\perp = 0$ with the notations of section III A. Then the variation of velocities should read $\delta \dot{q} = \dot{q} \cdot \delta \Theta(t) + q \cdot \delta \dot{\Theta}$. At the first order $(q + \delta q)^2 = R^2$ and $(q + \delta q) \cdot (\dot{q} + \delta \dot{q}) = 0$. The first variation of the lagrangian is therefore

$$\delta L = \frac{\partial L}{\partial q} \cdot (q \cdot \delta \Theta) + \frac{\partial L}{\partial \dot{q}} \cdot (\dot{q} \cdot \delta \Theta) + \frac{\partial L}{\partial \dot{\Theta}} \cdot (\dot{q} \cdot \delta \dot{\Theta}),$$

$$= \left( q \wedge \frac{\partial V}{\partial q} \right) \cdot \delta \Theta - m(q \wedge q) \cdot \delta \dot{\Theta},$$  

(27)

where we made use of equation (A8) and of the antisymmetry of the outer product. It follows that the variation of the action is

$$\delta S = \int_0^T dt \{ q \wedge \frac{\partial V}{\partial q} + m \frac{d}{dt} (q \wedge q) \} \cdot \delta \Theta,$$  

(28)

where the usual integration by part on time $t$ and the use of the boundary conditions at $t = 0$ and $t = T$ were made. Equation (28) can be rewritten in a more transparent way

$$\delta S = \int_0^T dt \{ -q \wedge f^\perp + \dot{K} \} \cdot \delta \Theta,$$  

(29)

where $K = mq \wedge \dot{q} = mR^2\Omega$ is the angular momentum of the particle. Demanding that $\delta S = 0$ for an arbitrary variation $\delta \Theta(t)$ does not automatically ensures that the bivector in brackets $A = -q \wedge f^\perp + \dot{K}$ in equation (29) vanishes. To see that, we decompose $A = A_\perp + A_\parallel$ as we did in section III A idem for $\delta \Theta$. We then note that $A \cdot \delta \Theta = \langle A, \delta \Theta \rangle_0 = A_\perp \cdot \delta \Theta_\perp + A_\parallel \cdot \delta \Theta_\par$. Since $\delta \Theta_\perp = 0$, we have simply $A \cdot \delta \Theta = \langle A_\parallel, \delta \Theta \rangle_0$. Now we expand $A_\parallel = \sum_i A_i e_i(\xi) \xi$ and $\delta \Theta(t) = \sum_i \delta \theta_i(t) e_i(\xi) \xi$ where the $\delta \theta_i(t)$ are arbitrary functions of time. Then the stationary condition says nothing about $A_\perp$ but implies that all the $A_i$ are zero. Therefore we have

$$-q \wedge f^\perp + \dot{K} = \sum_{i \neq j} c_{ij} e_i(\xi) e_j(\xi),$$  

(30)

where the coefficients $c_{ij}$ are unknown a priori. However since both $\dot{K} = q \wedge \dot{q}$ and $q \wedge f^\perp$ have a null projection onto the plane $E^d(\xi)$, it implies that all the $c_{ij}$ of equation (30) vanish.

Euler-Lagrange equation is thus

$$\dot{K} = mq \wedge \dot{q} = q \wedge f^\perp,$$
or, in term of the angular velocity
\[
\dot{\Omega} = \frac{1}{m} \xi \wedge f.
\] (31)

We recover the angular momentum theorem of equation (31). Note that taking the inner product of both sides of the above equation with vector \(q\) yields back the Newton equation (25) derived in section III A.

IV. ROLL : AN INTEGRATOR OF THE EQUATIONS OF MOTION ON A HYPERSPHERE

Let us begin with a short historical digression. The Verlet algorithm was originally devised to integrate numerically the Newton equations of motion of a system of \(N\) interacting point particles in the first MD simulations of simple classical fluids or plasmas [13]. The geometry considered in these pioneer works was the \(d = 3\) Euclidean space \(E^3\), within the usual and convenient periodic boundary conditions [12]. The so called velocity-Verlet algorithm derived later by Swiatek et al. is mathematically equivalent to that of Verlet but, numerically is more stable and precise [16]. SHAKE generalizes Verlet integration to systems of point particles with mechanical constraints, for instance molecules and polymers [14], while RATTLE generalizes the velocity-Verlet algorithm for the same class of systems [14]. The analysis of Andersen shows that RATTLE and SHAKE are not numerically equivalent [11]. It appears that SHAKE fails to consider hidden constraints on velocities which are correctly taken into account by RATTLE.

SHAKE or RATTLE can both be used to study the dynamic of particles confined on a hypersphere, but we consider only the superior RATTLE in appendix B. In next section IV A we derive ROLL from Taylor expansions of the equation of motion (25) (c.f. section IV A), and, in section IV B from the exact minimization of a discretized action.

A. Taylor expansions

1. ROLL-0

We first discretize equation of motion (25) and project it on hyperplane \(\xi^*_n\)
\[
P_{\xi^*_n} (\ddot{\xi}_n) = f^{\perp}_n / (mR),
\] (32)

which gives the projection of the acceleration at time \(t = nh\), where \(h\) denotes the time increment. This allows to approximate the positions at discrete times \(t_{n+1}\) with Taylor expansions :
\[
P_{\xi^*_n} (\xi_{n+1}) = +h\dot{\xi}_n + \frac{h^2}{2mR} f^{\perp}_n + \mathcal{O}(h^3),
\] (33a)
\[
P_{\xi^*_n} (\xi_{n-1}) = -h\dot{\xi}_n + \frac{h^2}{2mR} f^{\perp}_n + \mathcal{O}(h^3).
\] (33b)

Following Verlet and adding both equations gives us [13]
\[
P_{\xi^*_n} (\xi_{n+1}) = -P_{\xi^*_n} (\xi_{n-1}) + \frac{h^2}{mR} f^{\perp}_n + \mathcal{O}(h^4).
\] (34)

It is important to reckon that the knowledge of the projection \(P_{\xi^*} (\xi_{n+1})\) implies the full knowledge of the new position \(\xi_{n+1}\) of the particle at time \(t_{n+1}\). From equation (15) we have
\[
\xi_{n+1} = P_{\xi^*_n} (\xi_{n+1}) + \alpha \xi_n.
\] (35)

In order to satisfy the position constraint \(\xi^2_{n+1} = 1\) at time \(t_{n+1}\), the unknown parameter \(\alpha\) must be :
\[
\alpha = \pm \sqrt{1 - P_{\xi^*_n} (\xi_{n+1})^2}.
\] (36)

For a sufficient small time increment \(h\), \(\xi_n \cdot \xi_{n+1} > 0\) and the sign + should be retained. Therefore
\[
\xi_{n+1} = P_{\xi^*_n} (\xi_{n+1}) + \sqrt{1 - P_{\xi^*_n} (\xi_{n+1})^2} \xi_n.
\] (37)
Just as the Verlet algorithm, the integrator \(31\) says nothing about velocities at time \(t_{n+1}\), but generates a sequence of positions \(\xi_n\) on the hypersphere. As proposed by Verlet, velocities at time \(t_n\) can be obtained by subtracting equations \(33a\) and \(33a\) yielding

\[
\dot{\xi}_n = \frac{P_{\xi_n}(\xi_{n+1}) - P_{\xi_n}(\xi_{n-1})}{2h}.
\]  

Note that these expressions automatically satisfy the hidden constraint on velocities \(\xi_n \cdot \dot{\xi}_n = 0\).

To summarize, ROLL-0 is a discrete mapping \((\xi_{n-1}, \xi_n) \rightarrow \xi_{n+1}\) which can be written, for a sufficiently small time increment \(h\):

\[
P_{\xi_n}(\xi_{n+1}) = -P_{\xi_n}(\xi_{n-1}) + \frac{h^2}{mR} f_n^+ + O(h^3) ,
\]

\[
\xi_{n+1} = P_{\xi_n}(\xi_{n+1}) + \sqrt{1 - P_{\xi_n}(\xi_{n+1})^2} \xi_n ,
\]

\[
\dot{\xi}_n = \frac{P_{\xi_n}(\xi_{n+1}) - P_{\xi_n}(\xi_{n-1})}{2h} + O(h^2) ,
\]

it satisfies both constraints \(\xi_{n+1}^2 = 1\) and \(\xi_n \cdot \dot{\xi}_n = 0\).

2. ROLL-2

We skip ROLL-1 which will be derived in next section \([17]\) and we present now ROLL-2. We start from a Taylor expansion about time \(t_n\) rewritten with the help of bivector angular velocity \(\Omega_n\)

\[
\xi_{n+1} = \xi_n + h \xi_n \cdot \Omega_n + \frac{h^2}{2mR} f_n + O(h^3) .
\]

We project the equation on the tangent plane \(E_\xi^n\) obtaining

\[
P_{\xi_n}(\xi_{n+1}) = h \xi_n \cdot \Omega_n + \frac{h^2}{2mR} f_n + O(h^3)
\]

As explained in section \([17]\) \(P_{\xi_n}(\xi_{n+1})\) determines \(\xi_{n+1}\). We need an expression for \(\Omega_{n+1}\). In this aim we discretize equation \(31\) and adopt the velocity-Verlet recipe:

\[
\Omega_{n+1} = \Omega_n + \frac{h}{2mR} (\xi_{n+1} \wedge f_{n+1}^+ + \xi_n \wedge f_n^+) + O(h^2)
\]

To summarize, ROLL-2 is a discrete mapping \((\xi_n, \Omega_n) \rightarrow (\xi_{n+1}, \Omega_{n+1})\) which can be written, for a sufficiently small time increment \(h\):

\[
P_{\xi_n}(\xi_{n+1}) = h \xi_n \cdot \Omega_n + \frac{h^2}{2mR} f_n^+ + O(h^3) ,
\]

\[
\xi_{n+1} = P_{\xi_n}(\xi_{n+1}) + \sqrt{1 - P_{\xi_n}(\xi_{n+1})^2} \xi_n ,
\]

\[
\Omega_{n+1} = \Omega_n + \frac{h}{2mR} (\xi_{n+1} \wedge f_{n+1}^+ + \xi_n \wedge f_n^+) + O(h^2) .
\]

B. The discrete action: ROLL as a variational integrator

1. A variational integrator

We extend the analyses of Lee et al. concerning variational integrators of the discrete action on two-spheres \([2]\) to the case of hyperspheres of arbitrary dimension. Viewing Verlet integrator as an exact variational principle of a discrete action rather than the approximate Taylor expansion of exact equations of motion is an idea due to Marsden and collaborators, see e.g. reference \([17]\). Here it yields an unification of ROLL-0 and ROLL-2, lets us discover ROLL-1, and shows the mathematical equivalence of all these versions of ROLL.
As in section [V A] we consider only the case of one particle in the potential \( V(\xi) \) since the extension to \( N \) particles is trivial. The discrete lagrangian of the particle can be defined as \[ 17 \]

\[
\mathcal{L}_{d_n} = \frac{m R^2}{2 h} (\xi_{n+1} - \xi_n)^2 - \frac{h}{2} (V_n + V_{n+1}) ,
\]

where \( V_n \equiv V(\xi_n) \) is the total potential energy of the system in the configuration \( \xi_n \) and at discrete time \( t_n = nh \).

The discrete action between times \( t_0 = 0 \) and \( T = n_{\text{max}} h \) is defined as

\[
S = \sum_{n=0}^{n_{\text{max}} - 1} \mathcal{L}_{d_n}.
\]

We now compute the variation \( \delta S \) induced by some infinitesimal variation of the positions \( \delta \xi_n \). As in the continuous case discussed section [III B 2] we must be careful in the definition of \( \delta \xi_n \) and reckon that the configurational space is not a vector space but a group. Therefore, at each time \( t_n \), we consider an infinitesimal variation in the tangent \( n \)-plane \( \xi^*_n \): \( \delta \xi_n = \xi_n \cdot \delta \Theta_n \), where \( \delta \Theta_n \) is some bivector of the form \( \delta \Theta_n \equiv \delta \Theta^i_n = \sum_{1 \leq i \leq d} \epsilon_i (\xi_n) \wedge \xi_n \) where the scalars \( \epsilon_i \) are \( d \) arbitrary infinitesimal variations. As discussed in section [III B 2] this expansion of \( \delta \Theta_n \) ensures that the projection of bivector \( \delta \Theta_n \) in the tangent plane \( E^\perp_n \) is zero, in other words that \( \xi_n \wedge \delta \Theta_n = 0 \).

Discrete Hamilton’s principle states that \( \delta S = 0 \) for arbitrary \( \epsilon^i_n \) submitted to boundary conditions \( \epsilon^i_0 = \epsilon^i_{n_{\text{max}} - 1} = 0 \). The variation of the lagrangian is

\[
\delta \mathcal{L}_{d_n} = D\xi_n \mathcal{L}_{d_n} \cdot \delta \xi_n + D\xi_{n+1} \mathcal{L}_{d_n} \cdot \delta \xi_{n+1} ,
\]

where we have used Marsden’s notations \( D\xi_n = \partial/\partial \xi_n \) and \( D\xi_{n+1} = \partial/\partial \xi_{n+1} \). It follows from (46) and a discrete integration by parts, \( (i.e. \) a relabeling of the second sum), that the variation of the action is

\[
\delta S = \sum_{n=1}^{n_{\text{max}} - 1} \left[ D\xi_n \mathcal{L}_{d_n} + D\xi_{n+1} \mathcal{L}_{d_n} \right] \cdot \delta \xi_n ,
\]

where we made use of equation (48). The condition \( \delta S = 0 \) for an arbitrary \( \delta \Theta \) with the condition \( \xi_n \wedge \delta \Theta_n = 0 \) yields, as discussed at length in section [III B 2] to the equations

\[
\frac{m R^2}{h} \xi_n \wedge (\xi_{n-1} + \xi_{n+1}) = \xi_n \wedge f^\perp_n .
\]

After taking the inner product of both sides of (49) we obtain

\[
P_{\xi_n}(\xi_{n+1}) = -P_{\xi_n}(\xi_{n-1}) + \frac{h^2}{m R} f^\perp_n ,
\]

which is nothing , when complemented with equation (37), but the integrator ROLL-0 \((cf.\) equations 39).

2. linear and angular momenta

The linear momentum \( p_n \) is defined in the tangent plane \( E^d(\xi_n) \) as follows [8 17] :

\[
p_n \cdot \delta q_n = R \mathcal{P}_{q_n} \cdot \delta \xi_n = -D\xi_n \mathcal{L}_{d_n} \cdot \delta \xi_n
\]

This is satisfied for any \( \delta \xi_n \) perpendicular to \( \xi_n \), \( i.e. \) of the form \( \delta \xi_n = \xi_n \cdot \delta \Theta_n \) with \( \xi_n \wedge \delta \Theta_n = 0 \). Therefore we have

\[
p_n \cdot (\xi_n \cdot \delta \Theta_n) = \frac{1}{R} \left[ \frac{m R^2}{h} (\xi_{n+1} - \xi_n) + \frac{h}{2} \frac{\partial}{\partial \xi_n} V_n \right] \cdot (\xi_n \cdot \delta \Theta_n) .
\]
This equation must be satisfied for any $\delta \Theta_n \equiv \delta \Theta_n^\parallel$ and, following the same technique than in section IV B 1 we find after some algebra

\[ p_n = \frac{mR}{h} P_{\xi_n^\parallel} (\xi_{n+1}) - \frac{h}{2} f_n^\perp \quad (53a) \]

\[ \Omega_n \equiv \xi_n \wedge p_n / (mR) = \frac{1}{h} \xi_n \wedge \xi_{n+1} - \frac{h}{2mR} \xi_n \wedge f_n^\perp \quad (53b) \]

Similarly one defines the momentum $p_{n+1}$ as

\[ p_{n+1} = R p_n \cdot \delta q_n + f_{n+1}^\perp \quad (54) \]

and one obtains, with computations in the same vein as those used to compute $p_n$, the results

\[ \xi_{n+1} = P_{\xi_{n+1}^\parallel} (\xi_n) + \sqrt{1 - P_{\xi_{n+1}^\parallel} (\xi_n)^2} \xi_n \quad (55a) \]

\[ \Omega_{n+1} = \frac{1}{h} \xi_n \wedge \xi_{n+1} + \frac{h}{2mR} \xi_n \wedge f_{n+1}^\perp \quad (55b) \]

From equations (53a) and (55a) one obtains easily two versions of ROLL integrator.

- **ROLL-1**
  
  From equations (53a) and (55a) one obtains a discrete mapping $(\xi_n, p_n) \rightarrow (\xi_{n+1}, p_{n+1})$ which can be written, for a sufficiently small time increment $h$:

  \[ P_{\xi_n^\parallel} (\xi_{n+1}) = \frac{h}{mR} p_n + \frac{h^2}{2mR} f_n^\perp \quad (56a) \]

  \[ \xi_{n+1} = P_{\xi_{n+1}^\parallel} (\xi_n) + \sqrt{1 - P_{\xi_{n+1}^\parallel} (\xi_n)^2} \xi_n \quad (56b) \]

  \[ p_{n+1} = -\frac{mR}{h} P_{\xi_{n+1}^\parallel} (\xi_n) + \frac{h}{2} f_{n+1}^\perp \quad (56c) \]

  Equations (56) constitute ROLL-1 integrator. After defining $\dot{\xi}_n$ by the identity $p_n \equiv mR \dot{\xi}_n$, it turns out that there are identical to the equations (B10), constitutive of RATTLE algorithm, which are derived in appendix [13]

- **ROLL-2**
  
  From equations (53b) and (55b) one obtains a discrete mapping $(\xi_n, \Omega_n) \rightarrow (\xi_{n+1}, \Omega_{n+1})$ which is nothing but ROLL-2, derived in another way in section IV A 2 (cf equations (43)).

3. Properties of ROLL

It follows from the analysis of section IV B 1 that ROLL-1 and ROLL-2 are two mathematically equivalent integrators. ROLL-1 is also mathematically equivalent to RATTLE, therefore all these algorithms share the same properties and are thus reversible and symplectic, as shown for RATTLE in reference [11, 18]. In the case $d = 2$ it is a simple exercise to show that ROLL-2 coincides with the integrators of references [3, 4].

V. NUMERICAL APPLICATION

The main application of ROLL should be for MD simulations of simple fluids. Actually, the results of preceding sections can easily be extended to a system of $N$ particles. In case of pairwise additive potentials, for instance, the perpendicular force $f_n^\perp$ acting on particle "$\alpha$" can be written

\[ f_n^\perp = -\frac{1}{R} \sum_{\beta \neq \alpha} \frac{\partial v(\psi_{\alpha\beta})}{\partial \psi_{\alpha\beta}} t_{\alpha\beta}(\xi_\alpha) \quad (57) \]

where it had been recognized that the pair potential $v(\psi_{\alpha\beta})$ depends only on the geodesic distance $\psi_{\alpha\beta} = \cos^{-1} (\xi_\alpha \cdot \xi_\beta)$ on the unit hypersphere. In equation (57) $t_{\alpha\beta}(\xi_\alpha)$ denotes the tangent to the geodesic $\xi_\alpha$ at point $\xi_\alpha$ and orientated from $\xi_\alpha$ to $\xi_\beta$ [19, 20].
We applied the ROLL algorithm to MD simulations of the three dimensional version of the OCP. The OCP is a model which consists of identical point charges \( q \) of mass \( m \), immersed in a uniform neutralizing background of charge density \( \rho = -nq \) where \( n = N/V \) is the numerical density of particles \( V = 2\pi^2R^3 \) volume of the system \( 21, 22 \). In the thermodynamic limit, its properties depend on the sole dimensionless coupling parameter \( \Gamma = \beta q^2/a \) \( (\beta = 1/kT, \) \( T \) temperature, \( k \) Boltzmann constant, and \( a \) ion-sphere radius, defined in \( E^3 \), by \( a = (4\pi n/3)^{-1/3} \).

The expression for the configurational energy the OCP of in \( S^3(O,R) \) was derived in \( 23 \) and will not be repeated here. We only mention that the pair potential \( v(\psi) \) entering the configurational energy is essentially the electrostatic potential created by a point charge embedded in its neutralizing background. It is obtained by solving Poisson’s Equation analytically in \( S^3(O,R) \) \( 19, 20 \).

In reference \( 23 \) MC simulations in the canonical ensemble, performed on the hypersphere \( S^3(O,R) \), have produced very accurate results for the thermodynamic limit of the internal energy of the model with a relative precision \( p \sim 10^{-5} \) in the range \( 1 \leq \Gamma \leq 190 \). In these MC simulations the parameter \( \Gamma \) is fixed while, in the MD simulations, the total energy is fixed and the potential and kinetic energy (and therefore parameter \( \Gamma \)) must both be computed.

In our simulations we have chosen a system of units such that \( q = 1, m = 1, \) and \( a = 1 \). With this choice the unit of time, for instance is \( t = (k/2\pi\hbar) \), \( \hbar \) value of the time increment \( \hbar \sim 10^{-8} \) • 10^{-8}. Decreasing \( h \) to improve on the conservation of the total energy is not a good idea since then the phase space is not properly sampled. A more appealing analysis is probably to keep track of the extreme values of \( E/N \) during the run. We found \(-0.79814057 < E/N < -0.79814033 \) exemplifying the absence of drift and the excellent energy conservation for a quite long run of \( 7 \times 10^6 \) time steps.

A more extensive numerical study will be published elsewhere. A sample of \( N = 2000 \) ions was prepared in the state \( \Gamma \sim 30 \). We chose for the time increment \( \hbar = 0.01 \) (in reduced units). The initial state was prepared so that each of the 6 components of the total angular momentum bivector per particle was \( \sim 10^{-16} \). ROLL-2 ensures a perfect conservation of the angular velocity. With this respect ROLL-1 is slightly inferior because the angular velocities must be computed from the positions and the momenta yielding a slight loss in precision.

Figure 1 shows data for the instantaneous and cumulated potential (left) and total (right) energies per particle for a sub-run of \( 2 \times 10^5 \) steps. From the mean value of the kinetic energy we obtained the parameter \( \Gamma = 30.002(4) \). The reported statistical error, which corresponds to two standard deviations, was computed by dividing the run in \( n_h = 1400 \) blocs of 5000 time steps and was obtained by a standard block analysis \( 24 \).

\( \bullet \) \( < V > /N = -0.848137(5), \) \( \) i.e. a relative error of \( 6 \times 10^{-6} \). This value should be compared with the thermodynamic value \( < V > /N = -0.8481197(42) \) obtained in reference \( 23 \) by a finite size studies of MC simulations of the OCP at \( \Gamma = 30 \).

\( \bullet \) \( E/N = -0.798140454(4), \) \( \) i.e. a relative error of \( 5 \times 10^{-10} \). This error is of course strongly dependent on the value of the time increment \( h = 0.01 \). Decreasing \( h \) to improve on the conservation of the total energy is not a good idea since then the phase space is not properly sampled. A more appealing analysis is probably to keep track of the extreme values of \( E/N \) during the run. We found \(-0.79814057 < E/N < -0.79814033 \) exemplifying the absence of drift and the excellent energy conservation for a quite long run of \( 7 \times 10^6 \) time steps.
VI. CONCLUSION

We have presented in this article the symplectic integrator ROLL for MD simulations of simple fluids or plasmas on the hypersphere. It extends to hypersphere $S^d$ of arbitrary dimensions, notably $d = 3$, previous attempts made for 2-spheres [3, 4]. The use of GA theory plays an important role in this extension because, otherwise, it would be impossible to introduce angular velocities without resorting to awkward matricial representations. In the special case $d = 3$, an alternative to GA could be the use of quaternions. However, this would be only but a peculiar case of the more general approach given here, which is valid even for $d > 3$.

Preliminary tests in the case of the OCP demonstrated the validity of ROLL and applications to extensive numerical experiments on OCP and related models are under way.

Since GA is also a very powerful approach for the classical mechanics of rigid bodies [10], the extension of ROLL to molecular fluids is clearly possible. The rotations of bodies in the tangent plane $E^d_\xi$ could be described by the component $\Omega^\perp$ of the angular velocity set to zero for point particles. Applications to polar fluids and ionic solutions is appealing.

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Appendix A: Geometric Algebra

We give here a brief digest on geometric algebra. It is largely inspired by the introduction on GA given by Alan Macdonald in reference [8] as well as in his textbook [9].

The geometric algebra $\mathbb{G}^d$ is an extension of the inner product space $\mathbb{R}^d$ with more objects and operations. These objects are called multivectors. They can be added or multiplied by scalars of $\mathbb{R}$ and these two operations confer to $\mathbb{G}^d$ the structure of a vector space on the field $\mathbb{R}$. Note that $\mathbb{R}$ and $\mathbb{R}^d$ are vector subspaces of $\mathbb{G}^d$.

Moreover $\mathbb{G}^d$ is a graded algebra with a product named geometric product satisfying properties G0-G8, for all scalars $a$ and $A, B, C \in \mathbb{G}^n$.

G0. there is a 1.

G1. $A(B + C) = AB + BC$, $(B + C)A = BA + CA$.

G2. $(aB + C)A = A(aB) = a(AB)$.

G3. $(AB)C = A(BC)$, i.e. $\mathbb{G}^d$ is an associative but non commutative algebra.

G4. $A1 = A1 = A$.

G5. The geometric product of $\mathbb{G}^d$ is related to the scalar product of $\mathbb{G}^d$ by

$$uv = u \cdot u = |u|^2$$

for all vector $u \in \mathbb{R}$.

G6. Every orthogonal basis $\{e_i\}$, $i = 1 \ldots d$, for $\mathbb{R}^d$ determines a standard basis for the vector space $\mathbb{G}^d$. The $\binom{n}{k}$ multivectors $e_{i_1 \ldots i_k} = e_{i_1} \ldots e_{i_k}$ with $1 \leq i_1 < i_2 < \ldots < i_k \leq n$ are a basis for multivectors of grade $k$ or $k$-vectors. Therefore the dimension of $\mathbb{G}^d$ is $2^d$.

G7. Each multivector of the algebra $A$ can be uniquely expressed as a sum of $k$-vectors, $0 \leq k \leq n$, as $A = \langle A \rangle_0 + \langle A \rangle_1 + \ldots + \langle A \rangle_n$. Many results of GA are an extension of the fundamental identity

$$uv = u \cdot v + u \wedge v,$$

where $u \cdot v = \langle uv \rangle_0$ is the scalar or inner product of the two vectors $(u, v)$. Equation (A2) defines their outer product as $u \wedge v = \langle uv \rangle_2$. 


G8. More generally one defines the inner and outer products of a j-vector A and a k-vector B by the relations (they are non universal and we adopt those of Macdonald):

\[ A \cdot B = (AB)_{k-j} , \]  
\[ A \wedge B = (AB)_{k+j} . \]  

(A3a)  
\[ \text{(A3b)} \]

We end this short and necessarily incomplete digest by listing additional definitions and useful formula used in the main body of the paper.

P1. The outer product defined at equation \[(A3b)\] is associative, which allows to define unambiguously the wedge product of k arbitrary vectors \(u_1, \ldots, u_k \in \mathbb{R}\). One shows that

\[ u_1 \wedge u_2 \wedge \ldots \wedge u_k = \frac{1}{k!} \sum_P (-1)^{\sigma(P)} u_{P(1)} \ldots u_{P(2)} u_{P(k)} , \]

(A4)

where the sum runs on all permutations \(P\) of \((1, \ldots, k)\) of signature \(\sigma(P)\). The k-vector \(u_1 \wedge u_2 \wedge \ldots \wedge u_k\) is called a k-blade. For instance \(e_1 \wedge e_2 = e_1 e_2\). To distinguish k-blades from k-vectors we shall designate blades by bold math symbol (exception 1-vectors).

P2. \(I = e_1 e_2 \ldots e_d \equiv e_1 \wedge e_2 \wedge \ldots \wedge e_d\) is christened the pseudo-scalar of algebra \(G^d\). Note that \(I^{-1} = e_d \wedge e_{d-1} \wedge \ldots \wedge e_1 = (-1)^{\frac{d(d-1)}{2}} I\).

P3. The dual of a multivector \(A\) is defined as

\[ A^* = AI^{-1} . \]  
\[ \text{(A5)} \]

P4. If \(A\) is a k-blade (respect. \(A\) a k-vector) of \(G^d\) then \(A^*\) is a (n-k)blade (respect. \(A^*\) a (n-k)vector) of \(G^d\). For blades, we thus have a duality relation

\[ A^{**} = \pm A \]  
\[ \text{(A6)} \]

the sign depending on \(d\).

P5. A k-blade \(A\) represents a vector linear subspace of \(\mathbb{R}^d\) and its dual \(A^*\) the orthogonal complement. An orthogonal projection of an arbitrary multivector \(M\) on \(A\) can be expressed algebraically as

\[ P_A(M) = (M \cdot A) A^{-1} . \]  
\[ \text{(A7)} \]

P6. For arbitrary multivectors \(A, B, C\)

\[ A \cdot (B \cdot C) = (A \wedge B) \cdot C . \]  
\[ \text{(A8)} \]

Appendix B: Rattle algorithm

RATTLE numerical integration scheme of Newton equations \[(23a)\] consists in the discrete mapping \((\xi_n, \dot{\xi}_n) \mapsto (\xi_{n+1}, \dot{\xi}_{n+1})\). If applied to a particle constrained on a hypersphere it reads:

\[ \xi_{n+1} = \xi_n + h \dot{\xi}_n + \frac{h^2}{2mR} \{ f^\perp(\xi_n) - 2 \overline{\nabla} \xi_n \} + \mathcal{O}(h^3) \]  
\[ \dot{\xi}_{n+1} = \dot{\xi}_n + \frac{h}{2mR} \{ f^\perp(\xi_n) + f^\perp(\xi_{n+1}) - 2 \overline{\nabla} \dot{\xi}_n - 2 \overline{\nabla} \xi_n \} + \mathcal{O}(h^2) , \]

(B1a)  
\[ \text{(B1b)} \]

The two Legendre parameters \((\overline{\lambda}_r, \overline{\lambda}_s)\) are eliminated by solving the two constraint equations

\[ \xi_{n+1}^2 = 1 , \]  
\[ \xi_{n+1} \cdot \dot{\xi}_{n+1} = 0 . \]

(B2a)  
(B2b)

In the framework of RATTLE, two parameters \((\overline{\lambda}_r, \overline{\lambda}_s)\) are used to satisfy both position and velocity constraints \[(B2)\]; SHAKE requires only the constraint on position \[(B2a)\] and the hidden constraint on the velocity \[(B2b)\] is ignored.
We first take the scalar product of both sides of equation (B1a) with $\xi_n$. Since the constraints (B2) are fulfilled at time $t_n$ it yields readily
\[
\overline{\lambda}_r = \frac{mR}{h^2} \left(1 - \xi_n \cdot \xi_{n+1}\right). \quad (B3)
\]
Making use of expression (B3) in equation (B1a) yields
\[
P_{\xi_n^*} (\xi_{n+1}) = \hbar \dot{\xi}_n + \frac{\hbar^2}{2mR} f^\perp(\xi_n) + \mathcal{O}(h^3). \quad (B4)
\]
Recall that the position constraint (B2b) fully determines $\xi_{n+1}$, cf the discussion section IV A 1. For sufficiently small time increment $h$ one has
\[
\xi_{n+1} = P_{\xi_n^*} (\xi_{n+1}) + \sqrt{1 - P_{\xi_n^*} (\xi_{n+1})^2} \xi_n. \quad (B5)
\]
As expected, $\overline{\lambda}_r$ has disappeared from equation (B3) and moreover, for a sufficiently small $h$, $\overline{\lambda}_r$ is given by
\[
\overline{\lambda}_r = \frac{mR}{h^2} \sqrt{1 - P_{\xi_n^*} (\xi_{n+1})^2}. \quad (B6)
\]
With this choice for $\overline{\lambda}_r$, the particle stays on the sphere at all times.

In a following step, making use of the expression (B3) of $\overline{\lambda}_r$ in equation (B1b), we obtain a somehow simplified equation where only parameter $\overline{\lambda}_s$ survives
\[
\dot{\xi}_{n+1} = \frac{\xi_{n+1} - \xi_n}{h} + \frac{h}{2mR} \overline{\lambda}_s \{ f^\perp(\xi_{n+1}) - 2\overline{\lambda}_s \xi_{n+1}\} + \mathcal{O}(h^2). \quad (B7)
\]
Taking the scalar product of both sides with vector $\xi_{n+1}$ and imposing the two constraints (B2a) and (B2b) yields
\[
\overline{\lambda}_s = \frac{mR}{h^2} \left(1 - \xi_n \cdot \xi_{n+1}\right) = \overline{\lambda}_r. \quad (B8)
\]
With this choice for $\overline{\lambda}_s$ the velocity of the particle remains tangent to the hypersphere at all times. It is likely that the result $\overline{\lambda}_r = \overline{\lambda}_s$ is a peculiarity of the spherical geometry. Taking into account of expression (B8) for $\overline{\lambda}_s$, we can recast equation (B7) under the form
\[
\dot{\xi}_{n+1} = -\frac{1}{h} P_{\xi_{n+1}^*} (\xi_n) + \frac{h}{2mR} f^\perp(\xi_{n+1}) + \mathcal{O}(h^2), \quad (B9)
\]
where $P_{\xi_{n+1}^*} (\xi_n)$, the orthogonal projection of vector $\xi_n$ on the hyperplane $E^d(\xi_{n+1})$ perpendicular to $\xi_{n+1}$. Finally the RATTLE algorithm for the hypersphere $S^d$ can be summarized as
\[
P_{\xi_n^*} (\xi_{n+1}) = \hbar \dot{\xi}_n + \frac{\hbar^2}{2mR} f^\perp(\xi_n) + \mathcal{O}(h^3), \quad (B10a)
\]
\[
\xi_{n+1} = P_{\xi_n^*} (\xi_{n+1}) + \sqrt{1 - P_{\xi_n^*} (\xi_{n+1})^2} \xi_n, \quad (B10b)
\]
\[
\dot{\xi}_{n+1} = -\frac{1}{h} P_{\xi_{n+1}^*} (\xi_n) + \frac{h}{2mR} f^\perp(\xi_{n+1}) + \mathcal{O}(h^2). \quad (B10c)
\]
It turns out that the three equations (B10) are mathematically identical to those associated with algorithm ROLL-1, cf equations (20). We know from the mathematical study of reference [18] that RATTLE is reversible and symplectic. Therefore the same mathematical properties hold for ROLL.

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GA is a relatively new concept, with a lot of applications in many branches of physics, robotics and engineering. $\mathcal{G}^d$ is a Clifford algebra, the elements of which are called multi-vectors which represent subspaces of $\mathbb{R}^d$. The reader not acquainted with this subject will find a digest in appendix A and much more details in the recent review of A. Macdonald [8] and his remarkably clear elementary textbook [9]. At a more advanced level the reader should consult references [5, 7, 10]. For applications to physics the books [6, 10] will be consulted with profit. We adopt the notations and definitions of Macdonald throughout this paper.