

A Systematic Illustration on Reduction of N-body Problem with Application to Molecular Systems

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1. Introduction

N-body problem studies the dynamics of a given Lagrangian/Hamiltonian system in which N particles travel in \mathbb{R}^3 space with interactions described by a potential. The phase space could be viewed as \mathbb{R}^{6n} , since $T\mathbb{R}^{3n} \cong \mathbb{R}^{6n}$ and $T^*\mathbb{R}^{3n} \cong \mathbb{R}^{6n}$. This means that $6N$ possibly-nonlinear first order ODEs altogether describe the dynamics. It will be great if the dimension could be reduced. In fact, such idea was initiated by pioneer physicists ~400 years ago in solving Kepler problem [1, 2], in which the 2-body problem of sun-earth-gravity is studied with the aid of conservations of total linear momentum and total angular momentum.

Now, people could follow a systematic way to rigidly carry out reductions. Momentum maps are introduced to depict the essence of conserved quantities including total linear momentum and total angular momentum, and N-body problems could be studied by symplectic reduction theory which utilizes symmetries [3, 4, 5].

In this article, a geometrical reduction of 3-body problem will be described, with both the zero angular momentum and the non-zero angular momentum cases discussed. What follows is a discussion on the singularity issue associated with the reduction of 2-body problem. Then Yanao et al. [6]'s work of a further decrease of dimension in 6-body problem will be introduced and discussed. Applications and future directions will conclude the article.

2. Reduction of 3-body problem

2.1 Geometrical point of view

The configuration space is $Q = \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3$. The original phase space $M_0 = TQ$ has a dimension of 18. Consider the hyper-regular Lagrangian given as the sum of kinetic energy and an inter-particle potential energy:

$$L(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \dot{\mathbf{r}}_3) = \frac{1}{2}(m_1 \|\dot{\mathbf{r}}_1\|^2 + m_2 \|\dot{\mathbf{r}}_2\|^2 + m_3 \|\dot{\mathbf{r}}_3\|^2) - V(\|\mathbf{r}_1 - \mathbf{r}_2\|, \|\mathbf{r}_2 - \mathbf{r}_3\|, \|\mathbf{r}_3 - \mathbf{r}_1\|)$$

L has translational and rotational symmetries, i.e., it is both invariant under the action of the Lie algebra of translational group \mathbb{R}^3 and of rotational group $SO(3)$.

When the symmetry Lie group $G_1 = \mathbb{R}^3$, the Lie algebra $\mathfrak{g}_1 = \mathbb{R}^3$, $\mathfrak{g}_1^* \cong \mathbb{R}^3$, and the associated momentum map $J_1: TQ \rightarrow \mathfrak{g}_1^*$ is

$$J_1(v_q) = m_1 \dot{\mathbf{q}}_1 + m_2 \dot{\mathbf{q}}_2 + m_3 \dot{\mathbf{q}}_3, \text{ where } v_q = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \dot{\mathbf{q}}_1, \dot{\mathbf{q}}_2, \dot{\mathbf{q}}_3)$$

This corresponds to total linear momentum, which is conserved on any trajectory according to Noether's theorem.

When the symmetry Lie group $G_2 = SO(3)$, the Lie algebra $\mathfrak{g}_2 = \mathfrak{so}(3) \cong \mathbb{R}^3$, $\mathfrak{g}_2^* \cong \mathbb{R}^3$, and the associated momentum map $J_2 : TQ \rightarrow \mathfrak{g}_2^*$ is $J_2(v_q) = m_1 \dot{\mathbf{q}}_1 \times \mathbf{q}_1 + m_2 \dot{\mathbf{q}}_2 \times \mathbf{q}_2 + m_3 \dot{\mathbf{q}}_3 \times \mathbf{q}_3$

This corresponds to conserved total angular momentum.

Let's first employ symplectic reduction with respect to the translational symmetry $G_1 = \mathbb{R}^3$. Given a total linear momentum $\mu_1 \in \mathfrak{g}^* \cong \mathbb{R}^3$, $J_1^{-1}(\mu_1)$ will be a submanifold of TQ with codimension 3, if μ_1 is a regular value of J_1 . This means 3 variables could be reduced by fixing the total linear momentum to a certain value, since any value of μ_1 is regular in this case. The isotropy group $G_{\mu_1} = \{a \in G_1 \mid a \cdot \mu_1 = \mu_1\}$ stands for group actions that will not change the momentum. In this case, $G_{\mu_1} = G_1 = \mathbb{R}^3$, since none of the translation shifts will change the total linear momentum. $J_1^{-1}(\mu_1)/G_{\mu_1}$ is symplectic manifold with dimension of $18-3-3=12$ [3,4,5]. This could be understood as that centre of mass of the 3 particles is fixed at the origin of an inertial frame, since the total linear momentum is conserved. Another theorem guarantees that the reduced Hamiltonian system (we could freely switch between Lagrangian and Hamiltonian aspects since L is hyper-regular) corresponds to the original Hamiltonian system [3,4,5]. Therefore, the original system M_0 with 9 degrees of freedom (DOF for short) has been reduced to a system $M_1 = J_1^{-1}(\mu_1)/G_{\mu_1}$ with 6 DOF using the translational symmetry.

We now carry out the second symplectic reduction with respect to the rotational symmetry $G_2 = SO(3)$. Notice that M_1 could be identified with a submanifold of TQ , and the momentum map J_2 could be naturally inherited (we will therefore use the notation J_2 without any distinction). We could similarly reduce the phase space to $M_2 = J_2^{-1}(\mu_2)/G_{\mu_2}$, and relate the Hamiltonian flows. However, the second reduction is more complicated than the first one.

When $\mu_2 = 0$, $G_{\mu_2} = G_2 = SO(3)$, since any rotation will not change 0. However, the action of G_{μ_2} on $J_2^{-1}(0)$ is not free, since the action of $SO(3)$ on $T\mathbb{R}^3$ is not free and $(\mathbf{0}, \mathbf{0})$ is a fixed point. One way to overcome this is to introduce collision-free manifold \hat{M}_0 by getting rid of $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}_3$ points in M_0 , thus avoid fixed point in $J_2^{-1}(0) \subset M_1$. Notice the set of discarded points has a measure of 0. The dimension of M_2 will be $12-3-3=6$.

When $\mu_2 \neq 0$, G_{μ_2} is not $SO(3)$ but S^1 , since only rotations along the direction of the angular momentum could reserve it. The action of G_{μ_2} on $J_2^{-1}(\mu_2)$ is free (the particle position and velocity vector need to be on the same line, if fixed point existed; but this will result in $\mu_2 = 0$). The dimension of M_2 will be $12-3-1=8$.

I would like to make one more comment on the difference between the two reductions. The first reduction always and generally works, while the second doesn't. The difference intrinsically points out the fact that all inertial frames are equal while rotational frames are not!

2.2 Practical point of view

In this section we will choose local coordinates for the reduced system, as well as illustrate how to obtain the Lagrangian/Hamiltonian.

Since reduction with respect to translational symmetry corresponds to fixing an inertial frame at centre of mass, Jacobi vectors could be employed as coordinates [7, 8]. Of course, there are many choices other than Jacobi vectors, but Jacobi vectors is commonly used because it is a global coordinate which diagonalizes the kinetic energy for any value of N. “The usual way to define Jacobi coordinates is to organize the particles into a hierarchy of clusters, in which each cluster consists of one or more particles and where each Jacobi vector joins the centers of mass of two clusters, thereby creating a larger cluster.” [8] An easiest example is

$$\boldsymbol{\rho}_i = \sqrt{\mu_i} \left(\frac{\sum_{k=i}^{k=N} m_k \mathbf{r}_k}{\sum_{k=1}^{k=i} m_k} - \mathbf{r}_{i+1} \right), \forall i = 1, 2, \dots, N-1, \text{ where reduced mass } \mu_i = \frac{m_{i+1} \cdot \sum_{k=1}^i m_k}{\sum_{k=1}^{i+1} m_k}$$

It is obvious that Jacobi coordinates are invariant to translation of the original coordinates. If an extra vector of the position of centre of total mass \mathbf{p}_N , there is a diffeomorphism between $\{\boldsymbol{\rho}_i, \dot{\boldsymbol{\rho}}_i \mid i = 1, 2, \dots, N\}$ and $\{\mathbf{r}_i, \dot{\mathbf{r}}_i \mid i = 1, 2, \dots, N\}$. 3 DOF will be reduced.

On the other hand, how to construct coordinates of M_2 (called as shape coordinates) in the general n-body problem is a more intricate question. Eckart coordinates could be used, and some more recent literature studied this question too [9, 10]. For the N=3 case, there is a special set of coordinates (called shape coordinates) which treats the kinetic energy in a symmetrical way [7, 8]:

$$\begin{aligned} w_1 &= \|\boldsymbol{\rho}_1\|^2 - \|\boldsymbol{\rho}_2\|^2, \\ w_2 &= 2\boldsymbol{\rho}_1 \cdot \boldsymbol{\rho}_2, \\ w_3 &= 2\|\boldsymbol{\rho}_1 \times \boldsymbol{\rho}_2\|. \end{aligned}$$

Inner product and therefore the new shape coordinates are invariant to rotation. But this time it is not always true that 3 DOF could be reduced. We have shown this by a geometrical point of view, and we will see the same conclusion again in a second.

Using Jacobi vector, the kinetic energy could be written as:

$$K = \frac{1}{2} \|\boldsymbol{\mu}_1\|^2 \sum_{i=1}^N m_i + \frac{1}{2} \sum_{i=1}^{N-1} \|\boldsymbol{\rho}_i\|^2.$$

However, one will find out it is impossible to write the kinetic energy as a function of shape coordinates when $\boldsymbol{\mu}_2 \neq 0$, although it is possible when $\boldsymbol{\mu}_2 = 0$. For N=3, $\boldsymbol{\mu}_2 \neq 0$ case, we need one more variable which will help to construct the gauge potential part (defined in [8].) For N=3, $\boldsymbol{\mu}_2 = 0$ case, the kinetic energy is:

$$K = \frac{1}{2} \|\boldsymbol{\mu}_1\|^2 \sum_{i=1}^3 m_i + \frac{1}{2} \frac{\dot{w}_1^2 + \dot{w}_2^2 + \dot{w}_3^2}{4\sqrt{w_1^2 + w_2^2 + w_3^2}}$$

In this case, if the constant translational energy part is excluded, the kinetic

energy could be written as $g_{\mu\nu}\dot{q}^\mu\dot{q}^\nu$, where $q^i := w_i$, $(g_{\mu\nu}) = \frac{1}{4w} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$,

$w = \sqrt{w_1^2 + w_2^2 + w_3^2}$. Therefore, trajectories could be viewed as in Riemann space. Equation of motion could be written with a term of connection:

$$g_{\mu\nu}(\ddot{q}^\nu + \Gamma_{\kappa\lambda}^\nu \dot{q}^\kappa \dot{q}^\lambda) = -\frac{\partial V}{\partial q^\mu}, \text{ where } \Gamma_{\kappa\lambda}^\nu = \frac{1}{2} g^{\nu\mu} \left(\frac{\partial g_{\mu\kappa}}{\partial q^\lambda} + \frac{\partial g_{\mu\lambda}}{\partial q^\kappa} - \frac{\partial g_{\kappa\lambda}}{\partial q^\mu} \right) \text{ is the}$$

Christoffel symbol.

The task of writing potential energy lies in finding the relationship between $\|\mathbf{r}_{ij}\|, 1 \leq i < j \leq N$ and shape coordinates while no tangent (velocity) term is involved. The strategy is to use translational and rotational symmetries to simplify calculation.

When $N=3$, there are 3 inter-particle distances and 3 shape coordinates. Suppose the coordinates for the 3 particles are respectively $(0,0,0)$, $(a,b,0)$ and $(c,0,0)$, one could then calculate out both w_1, w_2, w_3 and $\|\mathbf{r}_{12}\|, \|\mathbf{r}_{23}\|, \|\mathbf{r}_{31}\|$ as functions of a, b, c . After eliminating a, b, c , one could obtain the mapping. The computation is very lengthy, but possible. The result when $m_1 : m_2 : m_3 = 1 : 1 : 0.1$ is:

$$r_{12} = \frac{\sqrt{-w_1 + \sqrt{w_1^2 + 21w_2^2 + 21w_3^2}}}{\sqrt{21}},$$

$$r_{23} = \frac{\sqrt{10w_1 - 21w_2 + 11\sqrt{w_1^2 + 21w_2^2 + 21w_3^2}}}{\sqrt{42}},$$

$$r_{31} = \frac{\sqrt{10w_1 + 21w_2 + 11\sqrt{w_1^2 + 21w_2^2 + 21w_3^2}}}{\sqrt{42}}.$$

Therefore, potential as a function of inter-particle distances can be written as a function of shape coordinates.

When $N=4$, there are 6 inter-particle distances and 6 shape coordinates. When $N=5$, there are 10 inter-particle distances and 9 shape coordinates. This is not a conflict, because since all particles lie in 3D Euclidean space, the 10 inter-particle distances are not all independent. Imagine Particle No.4's distances to particle No.1,2,3 are known, then Particle No.4 is fixed. Same for Particle No.5. Then there is no freedom in choosing Particle No.4 and No.5's distance. Of course, we omit all singular cases here.

In addition, other than direct calculation, we could also use chain rule to implicitly calculate $\frac{\partial V}{\partial w}$ and obtain the dynamics.

3. Reduction of 2-body problem

The dimension of the unreduced phase space in 2-body problem is 12. Suppose the same argument for 3-body problem applies, then 6 variables could be reduced due to

translational symmetry, and the other 6 variables could be reduced by rotational symmetry if total angular momentum is 0, which will result in no degree of freedom! This is of course absurd, since it is by no means guaranteed that the distance between two particles is fixed.

Before studying this seemingly paradox, let us review the traditional way of solving Kepler's problem [11], which is a 2-body problem with potential energy of $-\frac{Gm_1m_2}{\|\mathbf{r}_1 - \mathbf{r}_2\|}$. By fixing the center of mass to the origin, one obtains

$\mathbf{p}_1 = \mathbf{p}, \mathbf{p}_2 = -\mathbf{p}, \mathbf{r}_1 = \frac{m_2}{m_1 + m_2} \mathbf{r}, \mathbf{r}_2 = \frac{-m_1}{m_1 + m_2} \mathbf{r}$, and the problem has been transformed into

a 1-body problem:

$$\frac{d\mathbf{r}}{dt} = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\mathbf{p}^T,$$

$$\frac{d\mathbf{p}^T}{dt} = -\frac{Gm_1m_2}{\|\mathbf{r}\|^3} \mathbf{r}.$$

Then by using the conservation of angular momentum $\mathbf{r} \times \mathbf{p}^T = \mu_2$, one could introduce local coordinates (ρ, θ) by

$$\mathbf{r} = \rho \begin{pmatrix} \cos \theta \\ \sin \theta \\ 0 \end{pmatrix}, \mathbf{p} \frac{m_1 + m_2}{m_1 m_2} = \dot{\rho} \begin{pmatrix} \cos \theta & \sin \theta & 0 \end{pmatrix} + \rho \dot{\theta} \begin{pmatrix} -\sin \theta & \cos \theta & 0 \end{pmatrix}$$

And new equations of motion will be:

$$2\rho\dot{\theta} + \rho \frac{d\dot{\theta}}{dt} = 0$$

$$\frac{d\dot{\rho}}{dt} - \rho\dot{\theta}^2 + \frac{GM}{\rho^2} = 0$$

$$\frac{d\rho}{dt} = \dot{\rho}$$

$$\frac{d\theta}{dt} = \dot{\theta}$$

Most undergraduate-level textbooks will now conclude the problem saying the original system has been reduced to a four-dimensional system. But this is not end of the story.

The angular momentum μ_2 is a constant due to rotational symmetry. Suppose $\mu_2 = (c_1, c_2, c_3)$. By $\mathbf{r} \times \mathbf{p}^T = \mu_2$ we obtain:

$$(c_1, c_2, c_3) = \rho^2 \dot{\theta} (0, 0, 1) \quad (*)$$

Hence $\dot{\theta} = \frac{c_3}{\rho^2}$ and $\frac{d\dot{\theta}}{dt} = -2\frac{c_3}{\rho^3} \dot{\rho}$, and there are only 2 variables (i.e. 1 DOF) in the further reduced system.

Although translational reduction always works without singularity for any value of N , we again observe that rotational reduction doesn't. Why are 4 variables reduced by rotational symmetry, but not 6? An intuitive understanding could be obtained from (*), which tells c_1 and c_2 must be 0. Hence μ_2 being a constant vector could only give us one constraint instead of three constraints.

Notice different from $N=3$ case, only 4 variables could be reduced if the total angular momentum is 0. This is because 0 is not a regular value of the reduced $J_2 : T\mathbb{R}^3 \rightarrow g^*$ (since translation is excluded, this is the total angular momentum of 1-body problem), although G_{μ_2} are the same as in $N=3$ case. Regular symplectic reduction theorem's premise is not satisfied, and singular symplectic reduction is needed [5]. For reader's information, regular symplectic reduction theorem is listed here [4]:

Theorem: Let (P, ω) be a (weak) symplectic manifold on which the Lie group G acts symplectically and let $J : P \rightarrow g^*$ be an Ad^* -equivariant momentum mapping for this action. Assume $\mu \in g^*$ is a regular value of J and that the isotropy group G_μ under the Ad^* action on g^* acts freely and properly on $J^{-1}(\mu)$. Then $P_\mu = J^{-1}(\mu)/G_\mu$ has a unique (weak) symplectic form ω_μ with the property $\pi_\mu^* \omega_\mu = i_\mu^* \omega$, where $\pi_\mu : J^{-1}(\mu) \rightarrow P_\mu$ is the canonical projection and $i_\mu : J^{-1}(\mu) \rightarrow P$ is the inclusion.

Rotational reduction of non-zero total angular momentum case works exactly the same for $N=2$ and $N=3$.

4. 6-body problem

Same reduction as $N=3$ applies to $N>3$ cases, i.e. 12 / 10 dimensions could be reduced when total angular momentum is zero / non-zero. When N is large, we still need to face the high dimensionality ($6N-12$ or $6N-10$) of the phase space.

Yanao et al. [6] proposed a way to deal with this problem. Although the M6 cluster they focused on is 6-body problem with Morse potential, their method could be used for any $N>3$. After decomposing the $3 \times (N-1)$ -dimensional matrix

$W = (\mathbf{p}_1 \cdots \mathbf{p}_{(N-1)})$ by singular-value decomposition into the product of three matrices

$$W = RNU^T, \text{ where } R = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3), N = \begin{pmatrix} a_1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & a_2 & 0 & 0 & \cdots & 0 \\ 0 & 0 & a_3 & 0 & \cdots & 0 \end{pmatrix},$$

$U = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4, \cdots, \mathbf{u}_{n-1})$, the authors showed that 3 singular values a_1, a_2, a_3 serving as collective variables could largely characterize the dynamics features of six-atom Morse cluster. $a_1 \geq a_2 \geq a_3$ coincide with gyration radii and are related to the principle moments of inertia $M_3 \geq M_2 \geq M_1$ by $M_1 = a_2^2 + a_3^2, M_2 = a_3^2 + a_1^2, M_3 = a_1^2 + a_2^2$! The matrix R coincides with the principle-axis frame and thus specifies the instantaneous orientation of the system, while N and U determine the internal structure (size and symmetry). Other $3N-6-3$ or $3N-5-3$ shape coordinates obtained from U plus a_1, a_2, a_3 characterize the internal space.

Notice that when $N=3$, there are only two collective variables, which stand for a compression of information contained in w_1, w_2, w_3 obtained from reduction with respect to rotational symmetry. The rest of information is contained in U .

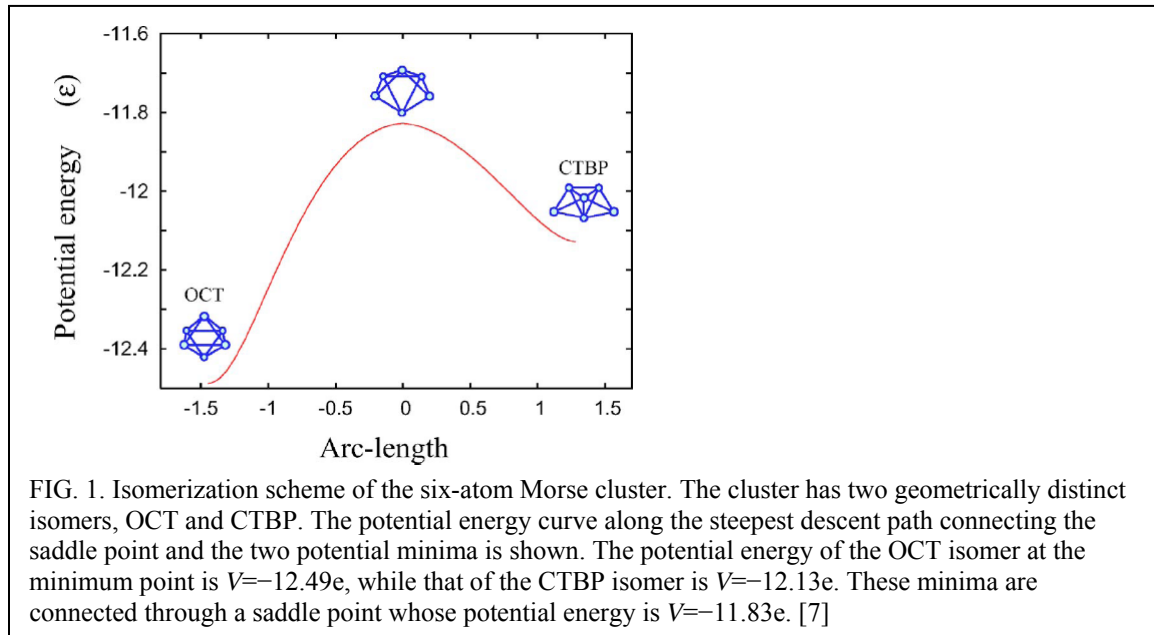
Although there is no geometrical explanation of this “reduction” so far, this heuristic way of reducing dimension is inspiring and has rich applications.

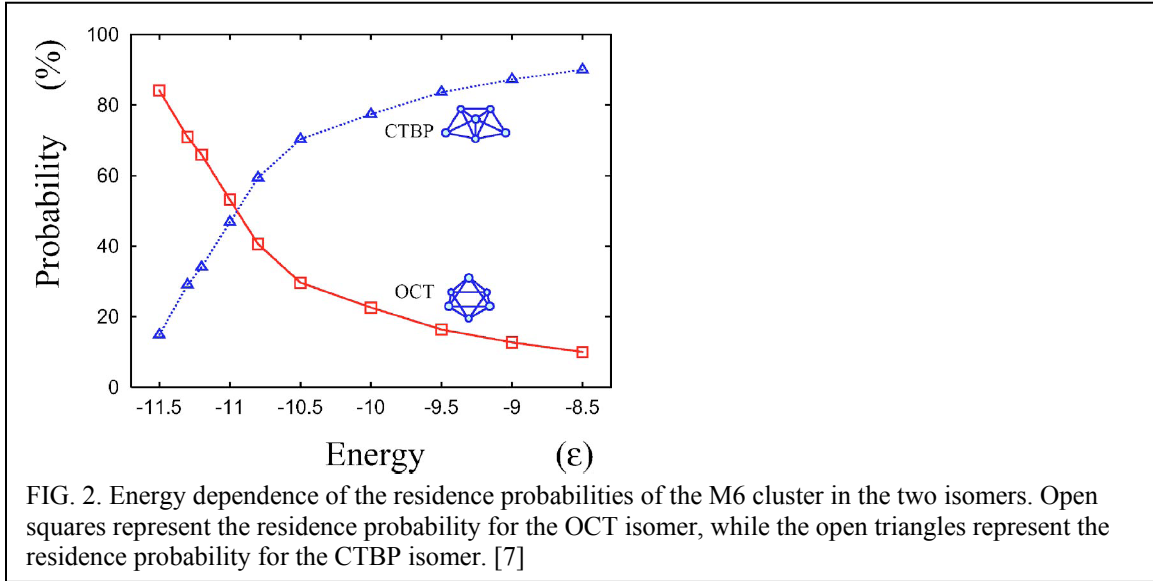
5. Applications to molecular systems and future directions

One important application is shown in Yanao et al. [6, 7], that is to use the reduced system to study the dynamics of molecule conformation switching under zero angular momentum assumption. To mimic Lennard-Jones potential, pairwise Morse potential is used:

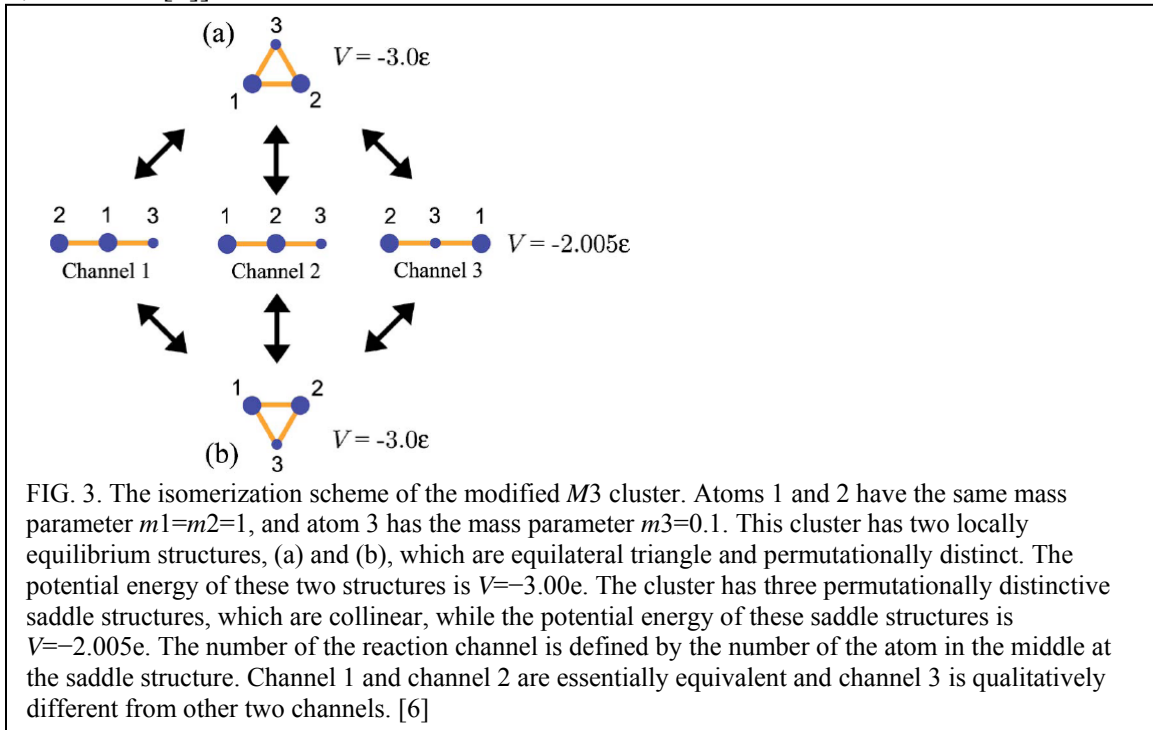
$$E_p = \sum_{i<j} [e^{-2(\|r_i-r_j\|-d_0)} - 2e^{-(\|r_i-r_j\|-d_0)}].$$

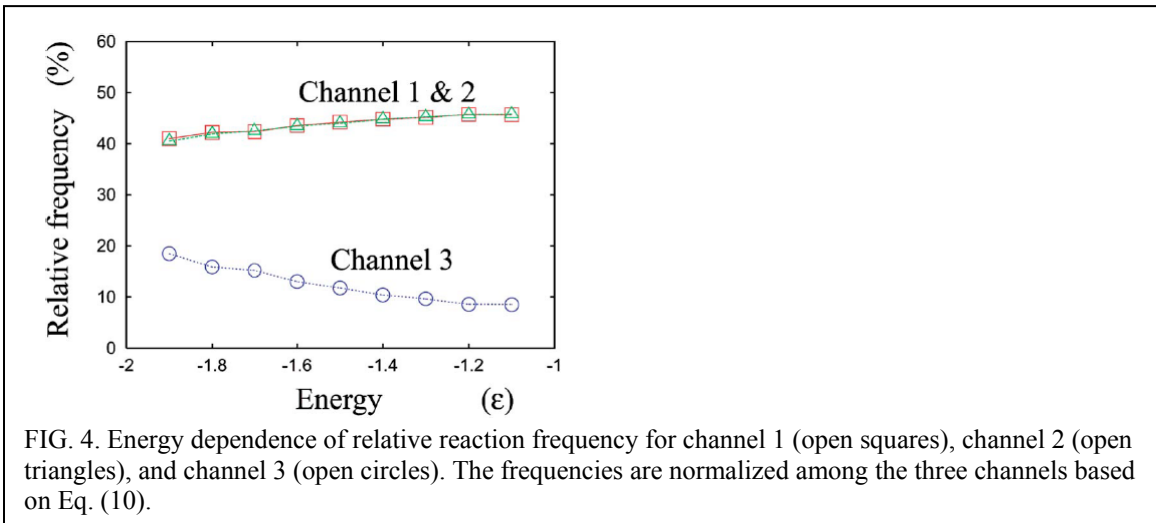
One microcanonical, constant energy simulation of the M6 cluster shows that certain conformation with higher potential energy is more favored than another conformation with lower potential energy [7] [FIG. 1,2].



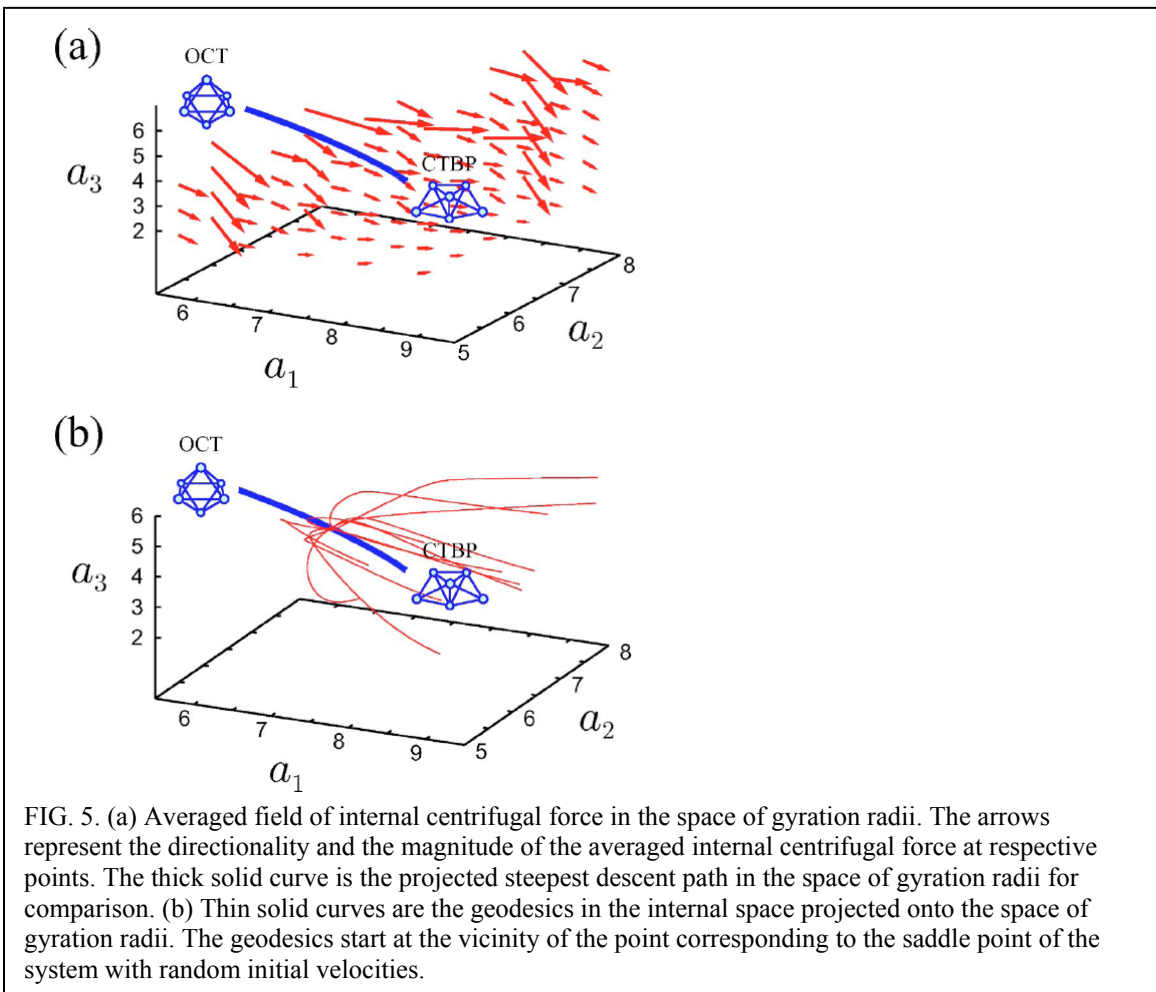


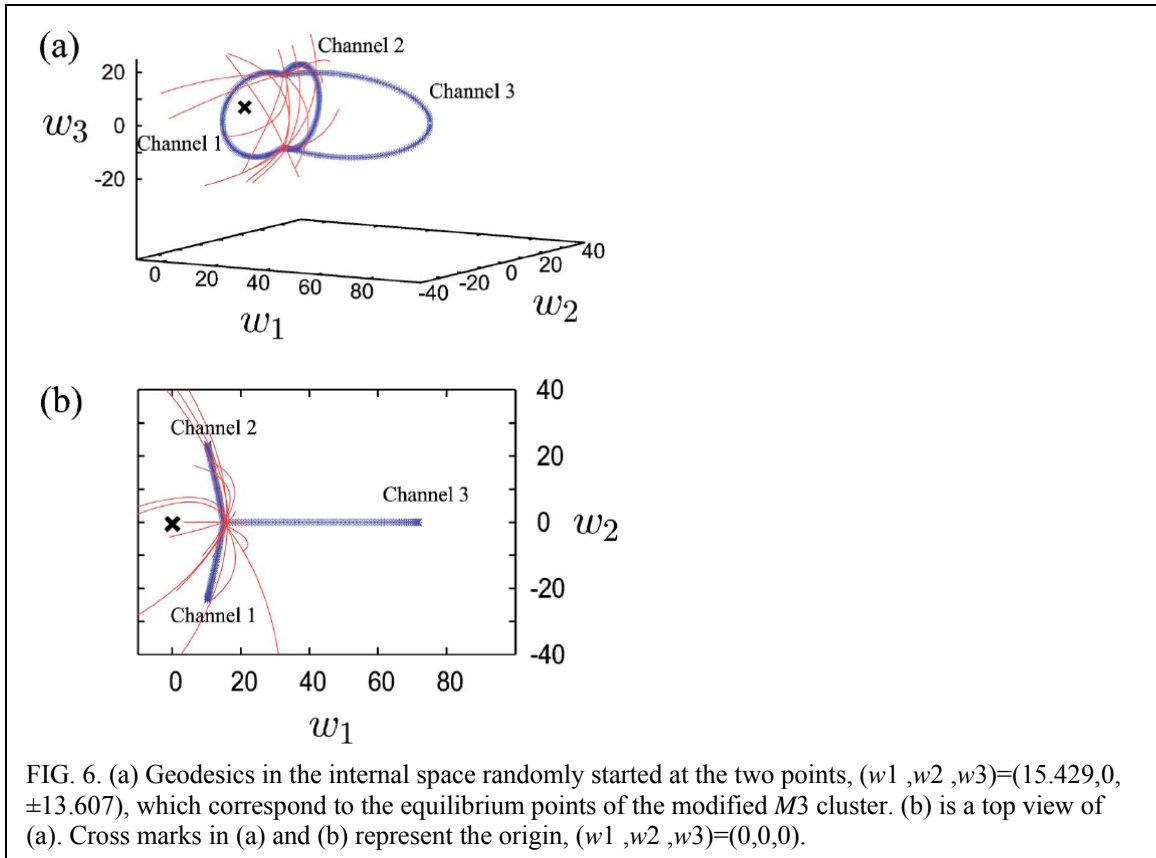
Another simulation of a tri-atomic system rediscovers that certain reaction pathways are more favored than other pathways [6] [renumbered as FIG. 3, FIG. 4; FIG. 1, FIG. 4 in [6]].





These two phenomena could be explained by the intrinsic geometry of the internal space. This is a mass effect, because the internal space geometry is related to the mass distributions. After averaging the force field, geodesics in the internal space are shown to favor these preferences! [renumbered FIG. 5, FIG. 6; FIG.4 in [6] and FIG. 6 in [7]].





Indeed, N-body reduction and internal space geometry provides a possible way to study molecules especially complex bio-molecules by first-principle. Ambitious topics include why suboptimal (and lethal!) but not optimal (in potential energy sense) conformation is preferred in prion protein (i.e., an explanation of mad cow disease), preference and switching within 3 different DNA helices, and much more. Yanao et al.'s work might just be the first step. In order to go along this road, many issues need to be studied.

One is the issue of numerical simulation. Since studied molecule might be very complex, the time span used in the simulation perhaps needs to be large, and numerical error might accumulate significantly. Variational integrator which preserves the symplectic structure could be employed given the Hamiltonian essence of the problem to attack.

Another direction is to relieve the unguaranteed assumption of zero total angular momentum. One extra DOF will be introduced, and quadratic cross terms between velocities and gauge potential will be added into the expression of kinetic energy, resulting in totally different Riemannian metric and geometry of the internal space.

Beside, complexity is a problem as crucial as the above ones, if not more. When N is large, translational and rotational reductions only helped a little and shape space is still of high dimension. On the other hand, three gyration of radii collective variables might be too coarse to depict fine structures of molecules. One approach is to generalize the singular value decomposition procedure used in extracting gyration of radii variables. More collective variables could be obtained if one heuristically embeds the Jacobi vectors

in higher dimension Euclidean spaces. However, it is hard to make any conclusion on the power of such “reduction” before doing experiments, since there is no geometrical or any other rigid explanation of such methodology so far.

On the other hand, probability and non-equilibrium statistical physics might play an important role in this subject. Besides working on the above issues, I am also verifying the hypothesis that certain conformation is favored because probability measure is concentrated there. This is not against Gibbs distribution, because other than the factor exponential to scaled minus potential energy, there is another factor measuring volume in the internal space.

Furthermore, concentration of measure phenomenon might provide a way to extract collective variables that could largely depict the internal spaces. This rigid interplay between analysis and geometry might shed new light on the reduction of N-body problem with large N.

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