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# Global methods in classical mechanics. The Euler–Lagrange equation

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Starting from a smooth manifold $Q$ as configurational space, the intrinsic form of Euler–Lagrange equation is derived using a differential geometrical approach in order to obtain a relation valid on the whole tangent bundle $TQ$ that constitutes the phase space of a generical mechanical system.

## 1. Introduction

Quantum mechanics is the main tool, among chemical physicist, to investigate molecular motions and transformations. Nevertheless, when the freedom degrees number of the system increases, quantum mechanical calculations become quite difficult to perform. In the last years, due to this kind of problem, classical mechanics is experiencing an increasing popularity for it is possible to perform calculations for many body problems and to obtain results in good agreement with experiments [2,4,7]. The problem of correspondence of classical to quantum mechanics has brought much discussion [3,9] and, at present, there does not exist a definitive answer.

Since Poincaré's pioneering work [10] it is well established that, generally, for a mechanical problem the phase space is a non-linear space. As a matter of fact, the mathematical model for mechanics consists of a smooth manifold that has a special geometrical structure called symplectic structure, together with a vector field [1]. This model admits a coordinate system only locally, and so it is more appropriate to use intrinsic methods to study a mechanical system.

In the present paper, after some brief preliminaries, the Euler–Lagrange equation, corner-stone of classical mechanics, is derived in the light of these methods. Useful applications of this approach to perform molecular dynamics simulations and analysis of vibrational spectra of polyatomic molecules will be the object of forthcoming papers.

## 2. Preliminaries

We review here, briefly, some basic concepts of differential geometry, referring the reader, for more details, to some texts on the argument [1,6].

### 2.1. Smooth manifolds

Let $M$ be a set and $m$ a positive integer. Any injection

$$\xi : U \subseteq M \to R^m$$

is called an *$m$-dimensional* (*local*) *chart* on $M$. Let

$$\xi : U \subseteq M \to R^m \quad \text{and} \quad \eta : V \to R^m$$

be two $m$-dimensional charts on $M$. They are said to be *$C^\infty$-related to each other* if $U \cap V = \emptyset$ or, when $U \cap V \neq \emptyset$, if their transitions functions

$$\eta \circ \xi^{-1} : \xi(U \cap V) \to R^m \quad \text{and} \quad \xi \circ \eta^{-1} : \eta(V \cap U) \to R^m$$

are $C^\infty$.

A collection $\mathcal{C}$ of $m$-dimensional charts is said to be an *$m$-dimensional atlas* on $M$ if the domains of the charts belonging to $\mathcal{C}$ are a covering of $M$.

An $m$-dimensional atlas $\mathcal{C}$ is said to be *$C^\infty$-differentiable* if, for every $\xi \in \mathcal{C}$, $\xi$ is $C^\infty$-related to every chart of $\mathcal{C}$.

An $m$-dimensional $C^\infty$-differentiable atlas $\mathcal{C}$ is said to be *complete* if each $m$-dimensional chart $C^\infty$-related to every chart of $\mathcal{C}$ belongs to $\mathcal{C}$.

A complete $m$-dimensional $C^\infty$-differentiable atlas is also called an *$m$-dimensional differential structure* on $M$.

A set $M$ equipped with an $m$-dimensional differential structure $\mathcal{A}$ is called an *$m$-dimensional smooth manifold*. All the charts of $\mathcal{A}$ are called *admissible charts* on $M$ and their domains are the *coordinate domains* on $M$.

### 2.2. Smooth mappings

Let $(M, \mathcal{A}_\mathcal{M})$ and $(N, \mathcal{A}_\mathcal{N})$ be smooth manifolds with $m = \dim M$ and $n = \dim N$ and

$$\Phi : M \to N$$

a mapping of $M$ in $N$. Let $p \in M$. If $\xi \in \mathcal{A}_\mathcal{M}$ is a chart with domain $U \ni p$ and $\eta \in \mathcal{A}_\mathcal{N}$ is a chart with domain $V \supseteq \Phi(U)$, the *coordinate expression* of $\Phi$ about $p$ is given by

$$\Phi_{\eta\xi} := \eta \circ \Phi \circ \xi^{-1} : \xi(U) \to R^n, \quad \xi(p) \to \eta\big(\Phi(p)\big).$$

$\Phi$ is said to be *$C^\infty$-differentiable* at $p$ if there exists a coordinate expression $\Phi_{\eta\xi}$ about $p$, which is $C^\infty$ at $\xi(p)$. $\Phi : M \to N$ is called a *smooth mapping* if it is $C^\infty$-differentiable at every point of $M$.

### 2.3. *Tangent space and tangent bundle*

Let $M$ be a smooth manifold, $FM$ the ring of real-valued smooth functions on $M$ and $p \in M$. Any $R$-linear map

$$v : FM \to R,$$

which obeys Leibnitz rule at $p$,

$$v(f, g) = v(f)g(p) + f(p)g(f) \quad (\forall f, g \in FM),$$

is called a derivation of $FM$ at $p$. Let $T_pM$ be the set of all the derivations of $FM$ at $p$. Putting, for any $f \in FM$,

$$(u + v)f := u(f) + v(f) \quad \text{and} \quad (av)f := av(f) \quad \forall a \in R,$$

$T_pM$ is given a structure of vector space. $T_pM$, endowed with the above structure, is called the *tangent space* of $M$ at $p$, and any $v \in T_pM$, a tangent vector of $M$ at $p$. It is easy to prove that dim $T_pM = \dim M$.

Let $TM$ be the disjoint union of all the tangent spaces of $M$. Any admissible chart on $M$ determines a $2m$-dimensional natural chart on $TM$. Natural charts set up a $2m$-dimensional differential structure on $TM$.

$TM$ – endowed with its natural differential structure – is called the *tangent bundle* of $M$.

### 2.4. *Cotangent space and cotangent bundle*

Let $M$ be a smooth manifold. At any $p \in M$, cotangent space $T_p^*M$ is the $m$-dimensional vector space, dual of $T_pM$, whose elements, called covectors, are the linear forms on $T_pM$. Let $T^*M$ be the disjoint union of all the cotangent spaces of $M$. Any admissible chart on $M$ determines a $2m$-dimensional natural chart on $T^*M$. Natural charts set up a $2m$-dimensional differential structure on $T^*M$.

$T^*M$ – endowed with its natural differential structure – is called the *cotangent bundle* of $M$.

### 2.5. *Smooth curves*

Let

$$\gamma : I \to M$$

be a smooth mapping of an open interval $I \subseteq R$ in a smooth manifold $M$. $\gamma$ is said to be a smooth curve, or *motion*, in $M$ and $\gamma(I)$ its *orbit*. The time derivative of $\gamma$ at $t \in I$, $\dot{\gamma}(t)$, is an element of $T_{\gamma(t)}M$. It is said to be the tangent vector of $\gamma$ at point $\gamma(t)$, or the *velocity* of $\gamma$ at instant $t$.

## 3. Geometrical tools

Let $M$ be a smooth manifold.

The tangent and cotangent bundle projections onto $M$ will be denoted by

$$\tau_M : TM \to M \quad \text{and} \quad \pi_M : T^*M \to M,$$

respectively. If

$$\Psi : M \to N$$

is a smooth mapping, then

$$T\Psi : TM \to TN$$

is the tangent mapping of $\Psi$. It satisfies the condition

$$\tau_N \circ T\Psi = \Psi \circ \tau_M.$$

The key role in the geometry of the tangent bundle $TM$ is played [5,8,11] by vertical lifting

$$\nu : TM \times_M TM \to TTM,$$

whose restriction $\nu_v$ to the fiber $(v) \times T_mM \cong T_mM$ over any $v \in TM$ (with $m = \tau_M(v)$) maps isomorphically $T_mM$ onto its own tangent space at $v$.

On the one hand, $\nu$ transforms the tangent mapping of $\tau_M$ into the almost tangent structure $S : TTM \to TTM$ defined, for any $v \in TM$, by

$$S_v := S|_{T_vTM} := \nu_v \circ T_v\tau_M.$$

On the other hand, $\nu$ transforms the identity mapping of $TM$ into the dilation vector field $\Delta : TM \to TTM$ defined, for any $v \in TM$, by

$$\Delta(v) := \nu_v(v).$$

The vertical tangent bundle $V\tau_Q$, defined as the set of all vectors $x \in TTM$ tangent to the fibres of $\tau_Q$, is then characterized by $S(x) = 0$.

The second tangent bundle $T^2M$, defined as the set of all vectors $x \in TTM$ satisfying $T\tau_M(x) = \tau_{TM}(x)$, is characterized by $S(x) = \Delta(\tau_{TM}(x))$.

The horizontal cotangent bundle $V^0\tau_M$, defined as the set of all covectors $\xi \in T^*TM$ annihilating $V\tau_M$, is characterized by $\xi \circ S_{\pi TM(\xi)} = 0$.

Moreover, we shall use the following vector bundle morphism:

$$\begin{array}{ccc} V^0\tau_M & \xrightarrow{\varpi_{\tau_M}} & T^*M \\ \Big\downarrow{\scriptstyle \pi_{TM}} & & \Big\downarrow{\scriptstyle \pi_M} \\ TM & \xrightarrow{\tau_M} & M \end{array}$$

where $\varpi_{\tau_M}$ is defined, for any $\xi \in V^0\tau_M$, by $\xi = \varpi_{\tau_M}(\xi) \circ T_v\tau_M$.

The restriction $V_v^\circ\tau_M \xrightarrow{\varpi_{\tau_M}} T_v\tau_M$ is a vector isomorphism.

## 4. The Euler–Lagrange equation

Let $(Q, L)$ denote an $n$-dimensional smooth manifold $Q$, endowed with a Lagrangian

$$L: P = TQ \to R,$$

that is, a real valued smooth function defined on the phase space $P$ of a mechanical system whose configurational space is $Q$. For any smooth curve

$$\gamma: I \to Q$$

($I \subseteq R$ being an open interval), the action integral in $(t_1, t_2) \subseteq I$ is given by

$$A_{t_2}^{t_1}(\gamma) := \int_{t_1}^{t_2} L \circ \dot{\gamma}\, \mathrm{d}t$$

(where $\dot{\gamma}: I \to TQ$ denotes the tangent lifting of $\gamma$).

In order to study the behaviour of $A_{t_2}^{t_1}(\gamma)$, when $\gamma$ is let to vary within a family of *nearby* smooth curves, we shall consider a smooth variation $(\varphi_s \circ \gamma)_{s\in R}$ of $\gamma$ defined by any one-parameter group $(\varphi_s)_{s\in R}$ of transformations of $Q$, whose infinitesimal generator $\zeta$ vanishes at $\gamma(t_1)$ and $\gamma(t_2)$. Recall that the tangent lifting of $\zeta$, i.e., the infinitesimal generator $Z$ of $(T\varphi_s)_{s\in R}$, is $\tau_Q$-related to $\zeta$ and satisfies

$$(SZ)_{\dot{\gamma}(t_i)} = \nu_{\dot{\gamma}(t_i)} \circ T_{\dot{\gamma}(t_i)}\tau_Q(Z_{\dot{\gamma}(t_i)}) = \nu_{\dot{\gamma}(t_i)}(\zeta_{\gamma(t_i)}) = 0.$$

Corresponding to the transformed curves $(\varphi_s \circ \gamma)_{s\in R}$, there is the action $s \to A_{t_1}^{t_2}(\varphi_s \circ \gamma)$, whose rate – starting from $\varphi_0 \circ \gamma = \gamma$ – is described by the first variation

$$\begin{aligned}
\left(\frac{\mathrm{d}}{\mathrm{d}s} A_{t_1}^{t_2}(\varphi_s \circ \gamma)\right)_{s=0} &= \int_{t_1}^{t_2} \left(\frac{\mathrm{d}}{\mathrm{d}s} L \circ T\varphi_s \circ \dot{\gamma}\right)_{s=0} \mathrm{d}t \\
&= \int_{t_1}^{t_2} \left\langle \left(\frac{\mathrm{d}}{\mathrm{d}s} T\varphi_s \circ \dot{\gamma}\right)_{s=0} \middle| \mathrm{d}L \circ \dot{\gamma} \right\rangle \mathrm{d}t \\
&= \int_{t_1}^{t_2} \langle Z|\mathrm{d}L\rangle \circ \dot{\gamma}\, \mathrm{d}t = \int_{t_1}^{t_2} ZL \circ \dot{\gamma}\, \mathrm{d}t = -\int_{t_1}^{t_2} [\widetilde{L}] \circ \ddot{\gamma} \cdot v(t)\, \mathrm{d}t
\end{aligned}$$

(using the Poincaré–Cartan 2-form associated with $L$, that is, $\omega := -\mathrm{d}\,\mathrm{d}_S L$). Here

$$v(t) := \left.\frac{\mathrm{d}q_s^h(t)}{\mathrm{d}s}\right|_{s=0} \left.\frac{\partial}{\partial q^h}\right|_{\gamma t} \in T_{\gamma(t)}Q$$

represents the tangent vector of curve $s \to (\varphi_s \circ \gamma)(t)$ at $(\varphi_0 \circ \gamma)(t) = \gamma(t)$ and

$$[\widetilde{L}] := \varpi_{\tau_Q} \circ [L],$$

$[L]$ being the Euler–Lagrange morphism defined by

$$[L]: T^2Q \to V^0\tau_Q, \quad x \to \mathrm{d}E_L\big(\tau(x)\big) -^\flat x,$$

where $E_L$ is the classical kinetic energy associated to $L$ and $^\flat$ is the musical morphism [1].

Now a smooth curve $\gamma : I \to Q$ is said to be a geodesic of $L$ if it satisfies Hamilton's variational principle of stationary action requiring

$$\left(\frac{\mathrm{d}}{\mathrm{d}s} A_{t_1}^{t_2}(\varphi_s \circ \gamma)\right)_{s=0} = 0$$

for each $(t_1, t_2) \subseteq I$ and each smooth variation $(\varphi_s \circ \gamma)_{s \in R}$, whose infinitesimal generator vanishes at $\gamma(t_1)$ and $\gamma(t_2)$.

**Lemma 1.** $[L] \circ \ddot{\gamma} = 0 \Leftrightarrow [\widetilde{L}] \circ \ddot{\gamma} = 0$.

*Proof.* It is sufficient to consider that $\varpi_{\tau_Q}$ is a vector isomorphism. □

**Theorem 2.** $\gamma$ is a geodesic of $(Q, L)$ if, and only if, $[L] \circ \ddot{\gamma} = 0$.

*Proof.* The *if* condition is trivial.

We shall prove the *only if* condition by the following *reductio ad absurdum*. Let $\gamma$ be a geodesic and $[L] \circ \ddot{\gamma}(t_0) \neq 0$ for some $t_0 \in I$. Let

$$\xi : U \to B_r^0$$

be a spherical chart with

$$\gamma(t_0) \in U \subseteq Q \quad \text{and} \quad x(t_0) := \xi\big(\gamma(t_0)\big) = 0 \in B_0^r \subseteq R^n.$$

Let's assume, e.g., $\lambda_1(t_0) > 0$ ($\lambda_h$, $h = 1, \ldots, n$, being the components of $[\widetilde{L}] \circ \ddot{\gamma}$ in $\xi$).

By continuity, we shall have

$$x(t) := \xi\big(\gamma(t)\big) \in B_0^{r/4} \quad \text{and} \quad \lambda_1(t) > 0$$

for each $t \in J$, $J$ being a suitably small open interval s.t. $t_0 \in J \subseteq I$. For each $t \in J$ and $s \in (-\varepsilon, \varepsilon)$ with $\varepsilon := r/8$, put

$$x_s(t) := x(t) + \big[s\big(\cos(t - t_0) - \cos\delta\big)\big]\delta_1$$

with $0 < \delta < \pi/2$ s.t. $(t_1, t_2) := (t_0 - \delta, t_0 + \delta) \subseteq J$ and $\delta_1$ first vector of canonical basis in $R^n$. Notice that (for each $t \in J$ and $s \in (-\varepsilon, \varepsilon)$)

$$\begin{aligned} x_s(t_0) &= \big[s(1 - \cos\delta)\big]\delta_1, \\ x_s(t) - x_s(t_0) &= x(t) + \big[s\big(\cos(t - t_0) - 1\big)\big]\delta_1, \end{aligned}$$

whence

$$\big|x_s(t_0)\big| = |1 - \cos\delta||s| < 2\left(\frac{r}{8}\right) = \frac{r}{4},$$

$$\left|x_s(t) - x_s(t_0)\right| \leqslant \left|x(t)\right| + \left|\cos(t - t_0) - 1\right||s| < \frac{r}{4} + \frac{r}{4} = \frac{r}{2},$$

and then

$$\left|x_s(t)\right| \leqslant \left|x_s(t) - x_s(t_0)\right| + \left|x_s(t_0)\right| < \frac{r}{2} + \frac{r}{4} < r,$$

that is, $x_s(t) \in B_0^r$ or, equivalently, $\gamma_s(t) := \xi^{-1}(x_s(t)) \in U$. This enables us to define a mapping

$$(s,t) \in (-\varepsilon, \varepsilon) \times J \to \gamma_s(t) \in U \subseteq Q,$$

which turns out to be a smooth variation of $\gamma$ with fixed end-points in $(t_1, t_2)$. The corresponding infinitesimal variation $v : J \to P$ has components in $\xi$ given, at each $t \in J$, by

$$\frac{\mathrm{d}}{\mathrm{d}s} x_s(t)\bigg|_{s=0} = \left[\cos(t - t_0) - \cos\delta\right]\delta_1,$$

that is,

$$v^1(t) = \cos(t - t_0) - \cos\ \delta,$$

positive in the interior and vanishing at the end-points of $(t_1, t_2)$ and

$$v^2(t) = \cdots = v^n(t) = 0,$$

therefore

$$\left(\frac{\mathrm{d}}{\mathrm{d}s} A_{t_1}^{t_2}(\varphi_s \circ \gamma)\right)_{s=0} = -\int_{t_1}^{t_2} \lambda_1 v^1\, \mathrm{d}t < 0. \qquad \square$$

So,

$$[L] \circ \ddot{\gamma} = 0 \tag{1}$$

is the *Euler–Lagrange equation* of geodesics and, for any motion $\gamma : I \to Q$, $[L] \circ \ddot{\gamma}$ is the geodesic curvature of $\gamma$.

In any admissible chart, that is, locally, Euler–Lagrange equation of geodesics is expressed by the classical equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}^h} - \frac{\partial L}{\partial q^h} = 0.$$

We would like to stress that equation (1) has been obtained starting from a generical Lagrangian that might be, for example, non-regular. Moreover, equation (1) is *intrinsic* in the sense that it does not depend on a locally valid coordinate system, but it works on the whole manifold, a natural place where it is possible to describe the motion of any mechanical system.

## 5. Conclusions

Classical mechanics can be a useful tool in a broad range of theoretical chemistry applications. Anyway, it has to be used in an adequate manner, keeping in mind that in most cases phase space is not linear and so admits a coordinate system only locally. Hence, intrinsic calculus of Cartan has to be preferred to conventional calculus of Newton.

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