HELMHOLTZ'S INVERSE PROBLEM OF THE DISCRETE CALCULUS OF VARIATIONS

by

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Abstract. — We derive the discrete version of the classical Helmholtz condition. Precisely, we state a theorem characterizing second order finite differences equations (see Definition 1) admitting a Lagrangian formulation. Moreover, in the affirmative case, we provide the class of all possible Lagrangian formulations.

Contents

1. Introduction

A classical problem in Analysis is the well-known *Helmholtz's inverse problem of the calculus of variations* (see [**6**, p.71], [**8**] and [**13**, p.377]): find a necessary and sufficient condition under which a (system of) differential equation(s) can be written as an Euler-Lagrange equation and, in the affirmative case, find all the possible Lagrangian formulations.

This problem has been studied by numerous authors and has been completely solved by A. Mayer [**12**] and A. Hirsch [**9, 10**]. The formulation that we use is due to V. Volterra [**14**]. Precisely, let O be a second order differential operator. Then, the differential equation $O(q) = 0$ can be written as a second order Euler-Lagrange equation if and only if all the Frechet derivatives of O are self-adjoint. This condition is usually called *Helmholtz condition.* We refer to [**13**] for a modern presentation and a complete proof of this theorem.

A more difficult problem is to deduce from this characterization a complete classification of second order differential equations admitting a variational formulation. This has been only solved in dimension three by J. Douglas in his seminal paper [**6**] following a previous work of D.R. Davis [**4, 5**]. We refer to [**6**, p.74-75] and [**13**, p.377-379] for a historical survey.

In recent years, an increasing activity has been devoted to a discrete version of the calculus of variations in the context of the geometric numerical integration. We refer to the book [**7**] and the review paper [**11**] for more details. In this context, a *second order discrete Euler-Lagrange equation* is given by:

$$\frac{\partial L_-}{\partial x}(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h) + \frac{\partial L_+}{\partial x}(\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h) \\ + \Delta_+ \left(\frac{\partial L_-}{\partial v}(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h) \right) - \Delta_- \left(\frac{\partial L_+}{\partial v}(\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h) \right) = 0, \quad (1)$$

for a given couple of Lagrangian (L_-, L_+) and where $\boldsymbol{T}$ is a bounded regular partition of $\mathbb{R}$ associated to the step size of discretization h. Δ_- (resp. Δ_+) is the backward (resp. forward) finite differences operator associated to $\boldsymbol{T}$.

In this framework, we formulate the *Helmholt'z inverse problem of the discrete calculus of variations* as follows: find a necessary and sufficient condition under which a second order finite differences equation (see Definition 1) can be written as a second order discrete Euler-Lagrange equation and, in the affirmative case, find all the possible Lagrangian formulations.

This problem has been studied by numerous authors. We refer in particular to the work of Albu-Opris [**1**] and Cracium-Opris [**3**]. However, in each of these papers, the structure of the proof follows a different scheme than the continuous case and does not allow to make comparisons. Moreover, we enlarge these studies by taking account of non autonomous finite differences equations.

2. Second order finite differences equations

2.1. Partitions and finite differences operators. — In the whole paper, let us consider the following set:

$$\mathbb{T} := \{ \boldsymbol{T} = (t_p)_{p=0,\dots,N} \in \mathbb{R}^{N+1} \text{ with } N \geq 4 \text{ and } \exists h > 0,\ \forall i = 0, \dots, N-1,\ t_{i+1} - t_i = h \}. \tag{2}$$

$\mathbb{T}$ is a set of bounded regular partitions $\boldsymbol{T}$ of $\mathbb{R}$. Hence, for any partition $\boldsymbol{T} \in \mathbb{T}$, an integer $N = \text{card}(\boldsymbol{T}) \geq 4$ and a step size of discretization $h > 0$ are associated. Consequently, for any $\boldsymbol{T} \in \mathbb{T}$, we can also associate the following *finite differences operators*:

$$\begin{array}{rccl} \Delta_- : & \mathbb{R}^{N+1} & \longrightarrow & \mathbb{R}^N \\ & \boldsymbol{Q} & \longmapsto & \left(\dfrac{Q_p - Q_{p-1}}{h} \right)_{p=1,\dots,N} \end{array} \tag{3}$$

and

$$\begin{array}{rccl} \Delta_+ : & \mathbb{R}^{N+1} & \longrightarrow & \mathbb{R}^N \\ & \boldsymbol{Q} & \longmapsto & \left(\dfrac{Q_p - Q_{p+1}}{h} \right)_{p=0,\dots,N-1} \end{array}. \tag{4}$$

Let us note that Δ_- (resp. $-\Delta_+$) is the classical backward (resp. forward) Euler approximation of the derivative operator d/dt. Moreover, Δ_- and $-\Delta_+$ commute and the discrete operator $-\Delta_+ \circ \Delta_-$ corresponds to the classical centered approximation of d^2/dt^2.

Let us remark that all these previous discrete elements depend on $\boldsymbol{T} \in \mathbb{T}$. For the reader's convenience, we omit this dependence in the notations.

In this paper, we are going to be interested in the discretization of differential equations defined on real intervals $[a,b]$. Hence, for any reals $a < b$, we introduce the following set:

$$\mathbb{T}_{a,b} := \{ \boldsymbol{T} \in \mathbb{T} \text{ with } 0 \leq t_0 - a < h \text{ and } 0 \leq b - t_N < h \}. \tag{5}$$

For any reals $a < b$, $\mathbb{T}_{a,b}$ is then a set of regular partitions $\boldsymbol{T}$ of the interval $[a,b]$.

2.2. Second order finite differences equations. — In the whole paper, let us note that we consider sufficiently smooth elements in order to make valid all the computations. The elements concerned are denoted by $\overline{O}$, $\overline{P}$, L, L_- and L_+.

In the continuous case, a second order differential equation on an interval $[a,b]$ is defined by $O^{a,b}(q) = 0$ where O is a second order differential operator, *i.e.*:

$$\begin{array}{rcccccl} O : & a < b & \longmapsto & O^{a,b} : & \mathscr{C}^2([a,b],\mathbb{R}) & \longrightarrow & \mathscr{C}^0([a,b],\mathbb{R}) \\ & & & & q & \longmapsto & O^{a,b}(q) \end{array} \tag{6}$$

with:

$$\begin{array}{rccl} O^{a,b}(q) : & [a,b] & \longrightarrow & \mathbb{R} \\ & t & \longmapsto & O^{a,b}(q)(t) = \overline{O}\big(q(t), \dot{q}(t), \ddot{q}(t), t\big) \end{array} \tag{7}$$

where $\dot{q}$ (resp. $\ddot{q}$) is the first (resp. second) derivative of q and where:

$$\begin{array}{rccl} \overline{O} : & \mathbb{R}^4 & \longrightarrow & \mathbb{R} \\ & (x,v,w,t) & \longmapsto & \overline{O}(x,v,w,t). \end{array} \tag{8}$$

Hence, a second order differential equation (independently of the interval $[a,b]$) is entirely determined by the application $\overline{O}$. Let us give the following discrete analogous definition:

Definition 1. — *A second order finite differences equation, associated to a partition $\boldsymbol{T} \in \mathbb{T}$, is defined by $P^{\boldsymbol{T}}(\boldsymbol{Q}) = 0$ where P is a second order finite differences operator, i.e.:*

$$\begin{array}{rcl} P: \ \boldsymbol{T} \in \mathbb{T} & \longmapsto & P^{\boldsymbol{T}}: \ \mathbb{R}^{N+1} \longrightarrow \mathbb{R}^{N-1} \\ & & \qquad \boldsymbol{Q} \longmapsto P^{\boldsymbol{T}}(\boldsymbol{Q}) = \big(P_p^{\boldsymbol{T}}(\boldsymbol{Q})\big)_{p=1,\dots,N-1} \end{array} \tag{9}$$

where

$$\forall p = 1, \dots, N-1, \ P_p^{\boldsymbol{T}}(\boldsymbol{Q}) = \overline{P}\big(Q_p, (\Delta_- \boldsymbol{Q})_p, (-\Delta_+ \boldsymbol{Q})_p, (-\Delta_+ \circ \Delta_- \boldsymbol{Q})_p, t_p, h\big) \tag{10}$$

and where

$$\begin{array}{rrcl} \overline{P}: & \mathbb{R}^5 \times \mathbb{R}_*^+ & \longrightarrow & \mathbb{R} \\ & (x, v_-, v_+, w, t, \xi) & \longmapsto & \overline{P}(x, v_-, v_+, w, t, \xi). \end{array} \tag{11}$$

A second order finite differences equation (independently of the partition $\boldsymbol{T} \in \mathbb{T}$) is then entirely determined by the application $\overline{P}$.

Let us consider a second order differential equation $O^{a,b}(q) = 0$ on an interval $[a, b]$. Then, a usual algebraic way in order to provide a discretization of this equation is to consider a partition $\boldsymbol{T} \in \mathbb{T}_{a,b}$ and to define:

$$\begin{array}{rrcl} \overline{P}: & \mathbb{R}^5 \times \mathbb{R}_*^+ & \longrightarrow & \mathbb{R} \\ & (x, v_-, v_+, w, t, \xi) & \longmapsto & \overline{O}\big(x, (1-\lambda)v_- + \lambda v_+, w, t\big) \end{array} \tag{12}$$

with $\lambda \in [0, 1]$. Hence, we obtain the numerical scheme $P^{\boldsymbol{T}}(\boldsymbol{Q}) = 0$. The parameter λ allows to choose for example the backward ($\lambda = 0$), centered ($\lambda = 1/2$) or forward ($\lambda = 1$) approximation of the derivative d/dt. Such a discretization of $O^{a,b}(q) = 0$ is said to be a *direct discretization.*

Example 1. — *Let us consider the Newton's equation with friction $q + \dot{q} + \ddot{q} = 0$ defined on a real interval $[a, b]$. It is a second order differential equation associated to $\overline{O}(x, v, w, t) = x + v + w$. Hence, considering $\lambda = 1/2$ and a partition $\boldsymbol{T} \in \mathbb{T}_{a,b}$, we obtain by direct discretization the following numerical scheme:*

$$\forall p = 1, \dots, N-1, \ Q_p + \frac{Q_{p+1} - Q_{p-1}}{2h} + \frac{Q_{p+1} - 2Q_p + Q_{p-1}}{h^2} = 0. \tag{13}$$

3. Formulation of the discrete version of the Helmholtz problem for second order finite differences equations

3.1. Reminder about the classical Helmholtz result for second order differential equations. — A continuous Lagrangian system derives from a variational principle. Precisely, let us consider two reals $a < b$ and the following Lagrangian functional:

$$\begin{array}{rrcl} \mathscr{L}^{a,b}: & \mathscr{C}^2([a,b], \mathbb{R}) & \longrightarrow & \mathbb{R} \\ & q & \longmapsto & \displaystyle\int_a^b L(q, \dot{q}, t)\, dt, \end{array} \tag{14}$$

where L is a Lagrangian, *i.e.* an application of the type:

$$\begin{array}{rrcl} L: & \mathbb{R}^3 & \longrightarrow & \mathbb{R} \\ & (x, v, t) & \longmapsto & L(x, v, t). \end{array} \tag{15}$$

Let $\mathscr{C}_0^2([a,b], \mathbb{R}) := \{w \in \mathscr{C}^2([a,b], \mathbb{R}), \ w(a) = w(b) = 0\}$ denote the set of *variations.* Then, $q \in \mathscr{C}^2([a,b], \mathbb{R})$ is said to be a *critical point* of $\mathscr{L}^{a,b}$ if for any variation w, we have

$D\mathscr{L}^{a,b}(q)(w) = 0$. A calculus of variations allows to characterize the critical points of $\mathscr{L}^{a,b}$ as the solutions on $[a,b]$ of the following *second order Euler-Lagrange equation*:

$$\frac{\partial L}{\partial x}(q,\dot{q},t) - \frac{d}{dt}\left(\frac{\partial L}{\partial v}(q,\dot{q},t)\right) = 0. \tag{EL^{a,b}}$$

A dynamical system governed by such an Euler-Lagrange equation is called *second order Lagrangian system*. We refer to [**2**, p.55-57] for more details concerning continuous Lagrangian systems.

The classical Helmholtz result is the following. Let O be a second order differential operator. The second order differential equation associated can be written as a second order Euler-Lagrange equation if and only if O satisfies the Helmholtz condition frequently given as the self-adjointness of all the Frechet derivatives of $O^{a,b}$ for any reals $a < b$. We refer to [**13**] for more details. Nevertheless, the Helmholtz condition can be more explicitly formulated: O satisfies the Helmholtz condition if and only if

$$\forall a < b,\ \forall q \in \mathscr{C}^2([a,b],\mathbb{R}),\ \frac{d}{dt}\left(\frac{\partial \overline{O}}{\partial w}(q,\dot{q},\ddot{q},t)\right) = \frac{\partial \overline{O}}{\partial v}(q,\dot{q},\ddot{q},t). \tag{H$_{\text{cont}}$}$$

3.2. Second order discrete Euler-Lagrange equations. — Let us give the discrete analogous definitions and results of the previous section:

Definition 2. — *A discrete Lagrangian functional, associated to a partition $\boldsymbol{T} \in \mathbb{T}$, is defined by:*

$$\begin{array}{rccl} \mathscr{L}^{\boldsymbol{T}}: & \mathbb{R}^{N+1} & \longrightarrow & \mathbb{R} \\ & \boldsymbol{Q} & \longmapsto & h\displaystyle\sum_{p=1}^{N} L_-\big(Q_p,(\Delta_-\boldsymbol{Q})_p,t_p,h\big) + h\sum_{p=0}^{N-1} L_+\big(Q_p,(-\Delta_+\boldsymbol{Q})_p,t_p,h\big), \end{array} \tag{16}$$

where (L_-,L_+) is a couple of Lagrangian, i.e. $L_\pm$ are applications of the type:

$$\begin{array}{rccl} L_\pm: & \mathbb{R}^3 \times \mathbb{R}^+_* & \longrightarrow & \mathbb{R} \\ & (x,v,t,\xi) & \longmapsto & L_\pm(x,v,t,\xi). \end{array} \tag{17}$$

Let $\mathbb{R}^{N+1}_0 := \{\boldsymbol{W} \in \mathbb{R}^{N+1},\ W_0 = W_N = 0\}$ denote the set of discrete variations. Then, $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ is said to be a discrete critical point of $\mathscr{L}^{\boldsymbol{T}}$ if for any discrete variation $\boldsymbol{W}$, we have $D\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = 0$.

A discrete calculus of variations allows to characterize the discrete critical points of $\mathscr{L}^{\boldsymbol{T}}$:

Theorem 3. — *Let (L_-,L_+) be a couple of Lagrangian and $\boldsymbol{T} \in \mathbb{T}$. Let $\mathscr{L}^{\boldsymbol{T}}$ be the discrete Lagrangian functional associated. Then, $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ is a discrete critical point of $\mathscr{L}^{\boldsymbol{T}}$ if and only if $\boldsymbol{Q}$ is solution of the following second order discrete Euler-Lagrange equation:*

$$\begin{multline} \frac{\partial L_-}{\partial x}(\boldsymbol{Q},\Delta_-\boldsymbol{Q},\boldsymbol{T},h) + \frac{\partial L_+}{\partial x}(\boldsymbol{Q},-\Delta_+\boldsymbol{Q},\boldsymbol{T},h) \\ + \Delta_+\left(\frac{\partial L_-}{\partial v}(\boldsymbol{Q},\Delta_-\boldsymbol{Q},\boldsymbol{T},h)\right) - \Delta_-\left(\frac{\partial L_+}{\partial v}(\boldsymbol{Q},-\Delta_+\boldsymbol{Q},\boldsymbol{T},h)\right) = 0. \end{multline} \tag{EL$^{\boldsymbol{T}}$}$$

A discrete dynamical system governed by such a discrete Euler-Lagrange equation is called second order discrete Lagrangian system.

Proof. — Let $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and $\boldsymbol{W} \in \mathbb{R}_0^{N+1}$. We have:

$$D\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h\sum_{p=1}^{N}\left[\frac{\partial L_-}{\partial x}(*_p)W_p + \frac{\partial L_-}{\partial v}(*_p)(\Delta_-\boldsymbol{W})_p\right] \\ + h\sum_{p=0}^{N-1}\left[\frac{\partial L_+}{\partial x}(**_p)W_p + \frac{\partial L_+}{\partial v}(**_p)(-\Delta_+\boldsymbol{W})_p\right] \quad (18)$$

where $* := (\boldsymbol{Q}, \Delta_-\boldsymbol{Q}, \boldsymbol{T}, h)$ and $** := (\boldsymbol{Q}, -\Delta_+\boldsymbol{Q}, \boldsymbol{T}, h)$. Let us remind the following *discrete integrations by part.* For any $(\boldsymbol{F}, \boldsymbol{G}) \in \mathbb{R}^{N+1} \times \mathbb{R}_0^{N+1}$, we have:

$$\sum_{p=1}^{N} F_p(\Delta_-\boldsymbol{G})_p = \sum_{p=1}^{N-1}(\Delta_+\boldsymbol{F})_p G_p \quad \text{and} \quad \sum_{p=0}^{N-1} F_p(\Delta_+\boldsymbol{G})_p = \sum_{p=1}^{N-1}(\Delta_-\boldsymbol{F})_p G_p. \quad (19)$$

Finally, combining (18) and (19), we obtain:

$$D\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h\sum_{p=1}^{N-1}\left[\frac{\partial L_-}{\partial x}(*_p) + \frac{\partial L_+}{\partial x}(**_p) + \Delta_+\left(\frac{\partial L_-}{\partial v}(*)\right)_p - \Delta_-\left(\frac{\partial L_+}{\partial v}(**)\right)_p\right] W_p, \quad (20)$$

which concludes the proof. □

Let us consider an Euler-Lagrange equation ($\mathrm{EL}^{a,b}$) defined on a real interval $[a, b]$ and L the Lagrangian associated. Let us take for example $L_-(x, v, t, \xi) = L(x, v, t)$ and $L_+ = 0$. Considering a partition $\boldsymbol{T} \in \mathbb{T}_{a,b}$, we obtain that $\mathscr{L}^{\boldsymbol{T}}$ is a discrete version of $\mathscr{L}^{a,b}$ and ($\mathrm{EL}^{\boldsymbol{T}}$) is obtained by discrete variational principle on $\mathscr{L}^{\boldsymbol{T}}$. Such a method leads ($\mathrm{EL}^{\boldsymbol{T}}$) to be called *variational integrator*: it is a numerical scheme for ($\mathrm{EL}^{a,b}$) having the particularity of preserving its intrinsic Lagrangian structure at the discrete level. We refer to [**7, 11**] for more details concerning the variational integrators. Let us note that one can also use a centered version by taking $L_-(x, v, t, \xi) = L_+(x, v, t, \xi) = L(x, v, t)/2$.

Example 2. — *Let us consider the Newton's equation without friction $q + \ddot{q} = 0$ defined on a real interval $[a, b]$. It is a second order differential equation associated to $\overline{O}(x, v, w, t) = x + w$ satisfying the continuous Helmholtz condition* ($\mathrm{H_{cont}}$)*. It corresponds to* ($\mathrm{EL}^{a,b}$) *with the quadratic Lagrangian $L(x, v, t) = (x^2 - v^2)/2$. Considering a partition $\boldsymbol{T} \in \mathbb{T}_{a,b}$, taking $L_-(x, v, t, \xi) = L(x, v, t)$ and $L_+ = 0$, we obtain the following discrete Euler-Lagrange equation:*

$$\forall p = 1, ..., N-1,\ Q_p + \frac{Q_{p+1} - 2Q_p + Q_{p-1}}{h^2} = 0. \quad (21)$$

Let us note that (21) *coincides with a direct discretization. Nevertheless, a direct discretization of an Euler-Lagrange equation do not lead necessary to a discrete Euler-Lagrange equation, see Example 4. In this case, we say that the Lagrangian structure is not preserved.*

3.3. Formulation of the discrete Helmholtz problem for second order finite differences equations. — Firstly, it is important to note that a second order discrete Euler-Lagrange equation is a second order finite differences equation (in the sense of Definition 1):

Proposition 4. — *Let (L_-, L_+) be a couple of Lagrangian. Then, the discrete Euler-Lagrange equation associated is a second order finite differences equation associated to:*

$$\begin{array}{rccl} \overline{P}: & \mathbb{R}^5 \times \mathbb{R}^+_* & \longrightarrow & \mathbb{R} \\ & (x, v_-, v_+, w, t, \xi) & \longmapsto & \displaystyle\sum_{i+j+k\geq 1} \Big[A_{i,j,k}(x, v_-, t, \xi) v_+^i + B_{i,j,k}(x, v_+, t, \xi) v_-^i \Big] w^j \end{array} \tag{22}$$

where

$$A_{i,j,k}(x,v,t,\xi) = \delta_{(i,j,k)=(0,0,1)} \frac{\partial L_-}{\partial x}(x,v,t,\xi) - \frac{\xi^{i+j+k-1}}{i!j!k!} \frac{\partial^{i+j+k+1} L_-}{\partial x^i \partial v^{j+1} \partial t^k}(x,v,t,\xi) \tag{23}$$

and where

$$B_{i,j,k}(x,v,t,\xi) = \delta_{(i,j,k)=(0,0,1)} \frac{\partial L_+}{\partial x}(x,v,t,\xi) + \frac{(-\xi)^{i+j+k-1}}{i!j!k!} \frac{\partial^{i+j+k+1} L_+}{\partial x^i \partial v^{j+1} \partial t^k}(x,v,t,\xi), \tag{24}$$

where δ is the Kronecker symbol.

Proof. — We have just to take a partition $\boldsymbol{T} \in \mathbb{T}$ and to develop $\partial L_- / \partial v$ and $\partial L_+ / \partial v$ in power series. □

We finally formulate the following discrete version of the Helmholtz problem:

Discrete Helmholtz problem for second order finite differences equations: *find a necessary and sufficient condition under which a second order finite differences equation can be written as a second order discrete Euler-Lagrange equation. Precisely, let P be a second order finite differences operator. Our aim is to find a necessary and sufficient condition on P under which there exists a couple of Lagrangian (L_-, L_+) such that for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$, we have:*

$$\begin{aligned} P^{\boldsymbol{T}}(\boldsymbol{Q}) = {} & \frac{\partial L_-}{\partial x}(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h) + \frac{\partial L_+}{\partial x}(\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h) \\ & + \Delta_+ \left(\frac{\partial L_-}{\partial v}(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h) \right) - \Delta_- \left(\frac{\partial L_+}{\partial v}(\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h) \right). \end{aligned} \tag{25}$$

4. Solution of the discrete Helmholtz problem for second order finite differences equations

Theorem 5. — *Let P be a second order finite differences operator. Then, the second order finite differences equation associated can be written as a second order discrete Euler-Lagrange equation if and only if P satisfies the following discrete Helmholtz condition:*

$$\forall \boldsymbol{T} \in \mathbb{T},\ \forall \boldsymbol{Q} \in \mathbb{R}^{N+1},\ \forall p = 2, ..., N-1,\ \Delta_- \left(\frac{\partial \overline{P}}{\partial w}(\star) \right)_p = \frac{\partial \overline{P}}{\partial v_-}(\star_p) + \frac{\partial \overline{P}}{\partial v_+}(\star_{p-1}), \tag{$\mathrm{H}_{\mathrm{disc}}$}$$

where $\star := \big(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, (-\Delta_+ \boldsymbol{Q}), (-\Delta_- \circ \Delta_- \boldsymbol{Q}), \boldsymbol{T}, h \big)$.

Proof. — See Sections 5 and 6. □

Let us note the similarity between the classical Helmholtz condition ($\mathrm{H}_{\mathrm{cont}}$) and its discrete version ($\mathrm{H}_{\mathrm{disc}}$). It is also important to note that, similarly to the continuous case, the discrete Helmholtz condition ($\mathrm{H}_{\mathrm{disc}}$) corresponds to the self-adjointness of all the Frechet derivatives of $P^{\boldsymbol{T}}$ for any $\boldsymbol{T} \in \mathbb{T}$, see Section 5.

Example 3. — *Let us take the second order finite differences equation* (21) *obtained in Example 2. It is associated to the application* $\overline{P}(x, v_-, v_+, w, t, \xi) = x + w$ *which satisfies the discrete Helmholtz condition* $(\mathrm{H}_{\mathrm{disc}})$*. It is expected because* (21) *is a discrete Euler-Lagrange equation by construction.*

Example 4. — *Let us consider the differential equation* $q + \sin(\dot{q})\ddot{q} = 0$ *defined on a real interval* $[a, b]$*. It is a second order differential equation associated to the application* $\overline{O}(x, v, w, t) = x + \sin(v)w$ *satisfying* $(\mathrm{H}_{\mathrm{cont}})$*. It corresponds to* $(\mathrm{EL}^{a,b})$ *associated to the Lagrangian* $L(x, v, t) = (x^2/2) + \cos(v)$*. Let us consider* $\boldsymbol{T} \in \mathbb{T}_{a,b}$ *and define* $\overline{P}(x, v_-, v_+, w, t, \xi) = \overline{O}\big(x, (1-\lambda)v_- + \lambda v_+, w, t\big)$ *with* $\lambda \in [0, 1]$*. Then, we obtain by direct discretization the following second order finite differences equation:*

$$\forall p = 1, ..., N-1,\ Q_p + \sin\left(\frac{\lambda Q_{p+1} + (1-2\lambda)Q_p + (\lambda - 1)Q_{p-1}}{h}\right)\frac{Q_{p+1} - 2Q_p + Q_{p-1}}{h^2} = 0. \tag{26}$$

Let P *be the second order finite differences operator associated. Then,* P *does not satisfy* $(\mathrm{H}_{\mathrm{disc}})$ *and consequently* (26) *can not be written as a second order discrete Euler-Lagrange equation. This is an example of direct discretization of an Euler-Lagrange equation not leading to a discrete Euler-Lagrange equation. The numerical scheme* (26) *does not preserve the Lagrangian structure of the differential equation at the discrete level.*

5. Discrete Helmholtz condition and self-adjointness of Frechet derivatives of second order finite differences operator

In this section, we prove that a second order differences operator P satisfies the discrete Helmholtz condition $(\mathrm{H}_{\mathrm{disc}})$ if and only if all the Frechet derivatives of $P^{\boldsymbol{T}}$ are self-adjoint for any $\boldsymbol{T} \in \mathbb{T}$.

5.1. Properties of the discrete derivative operators. — In this section, we first remind the classical discrete versions of the integration by part and the Leibniz formula.

***Lemma 6* (Discrete Leibniz formulas).** — *Let* $\boldsymbol{T} \in \mathbb{T}$ *and* $\boldsymbol{Q}$*,* $\boldsymbol{W} \in \mathbb{R}^{N+1}$*. Then, we have:*

$$\forall p = 1, ..., N,\ \ (\Delta_- \boldsymbol{Q}\boldsymbol{W})_p = (\Delta_- \boldsymbol{Q})_p W_p + Q_{p-1}(\Delta_- \boldsymbol{W})_p \tag{27}$$

and

$$\forall p = 0, ..., N-1,\ \ (\Delta_+ \boldsymbol{Q}\boldsymbol{W})_p = (\Delta_+ \boldsymbol{Q})_p W_p + Q_{p+1}(\Delta_+ \boldsymbol{W})_p. \tag{28}$$

Finally, for any $p = 1, ..., N-1$*, we have:*

$$\begin{aligned}(-\Delta_+ \circ \Delta_- \boldsymbol{Q}\boldsymbol{W})_p = (-\Delta_+ \circ \Delta_- \boldsymbol{Q})_p W_p + \boldsymbol{Q}_p(-\Delta_+ \circ \Delta_- \boldsymbol{W})_p \\ + (-\Delta_+ \boldsymbol{Q})_p(-\Delta_+ \boldsymbol{W})_p + (\Delta_- \boldsymbol{Q})_p(\Delta_- \boldsymbol{W})_p.\end{aligned} \tag{29}$$

For any $\boldsymbol{T} \in \mathbb{T}$, let us denote $\mathbb{R}^{N+1}_{0,0} := \{\boldsymbol{W} \in \mathbb{R}^{N+1},\ W_0 = W_1 = W_{N-1} = W_N = 0\}$.

***Lemma 7* (Discrete integrations by part).** — *Let* $\boldsymbol{T} \in \mathbb{T}$ *and* $(\boldsymbol{Q}, \boldsymbol{W}) \in \mathbb{R}^{N+1} \times \mathbb{R}^{N+1}_{0,0}$*. Then, we have:*

$$\sum_{p=1}^{N-1} Q_p(\Delta_- \boldsymbol{W})_p = \sum_{p=2}^{N-2} (\Delta_+ \boldsymbol{Q})_p W_p, \quad \textit{and} \quad \sum_{p=1}^{N-1} Q_p(\Delta_+ \boldsymbol{W})_p = \sum_{p=2}^{N-2} (\Delta_- \boldsymbol{Q})_p W_p. \tag{30}$$

Finally, we have:

$$\sum_{p=1}^{N-1} Q_p(-\Delta_+ \circ \Delta_- \boldsymbol{W})_p = \sum_{p=2}^{N-2} (-\Delta_+ \circ \Delta_- \boldsymbol{Q})_p W_p. \tag{31}$$

5.2. Interpretation of the discrete Helmholtz condition as self-adjointness of Frechet derivatives of second order finite differences operator. — Let us define the following discrete version of the self-adjointness of a Frechet derivative for a differential operator:

Definition 8. — *Let P be a second order finite differences operator, $\boldsymbol{T} \in \mathbb{T}$ and $\boldsymbol{Q} \in \mathbb{R}^{N+1}$. We denote by $DP^{\boldsymbol{T}}(\boldsymbol{Q})$ the Frechet derivative of $P^{\boldsymbol{T}}$ at the point $\boldsymbol{Q}$. Finally, we denote by $DP^{\boldsymbol{T}}(\boldsymbol{Q})^*$ the adjoint of $DP^{\boldsymbol{T}}(\boldsymbol{Q})$ defined by:*

$$\begin{array}{rccl} DP^{\boldsymbol{T}}(\boldsymbol{Q})^* : & \mathbb{R}^{N+1} & \longrightarrow & \mathbb{R}^{N-3} \\ & \boldsymbol{Z} & \longmapsto & DP^{\boldsymbol{T}}(\boldsymbol{Q})^*(\boldsymbol{Z}) = \big(DP_p^{\boldsymbol{T}}(\boldsymbol{Q})^*(\boldsymbol{Z})\big)_{p=2,\dots,N-2} \end{array} \tag{32}$$

satisfying:

$$\forall (\boldsymbol{W},\boldsymbol{Z}) \in \mathbb{R}^{N+1}_{0,0} \times \mathbb{R}^{N+1},\ h\sum_{p=1}^{N-1} DP_p^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W})Z_p = h\sum_{p=2}^{N-2} DP_p^{\boldsymbol{T}}(\boldsymbol{Q})^*(\boldsymbol{Z})W_p. \tag{33}$$

Finally, $DP^{\boldsymbol{T}}(\boldsymbol{Q})$ is said to be self-adjoint if for any $p = 2,\dots,N-2$, $DP_p^{\boldsymbol{T}}(\boldsymbol{Q}) = DP_p^{\boldsymbol{T}}(\boldsymbol{Q})^*$.

First, a simple calculation leads to the following result:

Proposition 9. — *Let P be a second order finite differences operator, $\boldsymbol{T} \in \mathbb{T}$ and $\boldsymbol{Q} \in \mathbb{R}^{N+1}$. Then, for any $p = 1,\dots,N-1$ and any $\boldsymbol{W} \in \mathbb{R}^{N+1}$, we have:*

$$DP_p^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = \frac{\partial \overline{P}}{\partial x}(\star_p)W_p + \frac{\partial \overline{P}}{\partial v_-}(\star_p)(\Delta_-\boldsymbol{W})_p + \frac{\partial \overline{P}}{\partial v_+}(\star_p)(-\Delta_+\boldsymbol{W})_p + \frac{\partial \overline{P}}{\partial w}(\star_p)(-\Delta_+\circ\Delta_-\boldsymbol{W})_p, \tag{34}$$

where $\star := \big(\boldsymbol{Q}, \Delta_-\boldsymbol{Q}, (-\Delta_+\boldsymbol{Q}), (-\Delta_-\circ\Delta_-\boldsymbol{Q}), \boldsymbol{T}, h\big)$.

Then, applying Lemmas 6 and 7 in Proposition 9, we can give explicitly the adjoint of a Frechet derivative:

Proposition 10. — *Let P be a second order finite differences operator, $\boldsymbol{T} \in \mathbb{T}$ and $\boldsymbol{Q} \in \mathbb{R}^{N+1}$. Then, for any $p = 2,\dots,N-2$ and any $\boldsymbol{W} \in \mathbb{R}^{N+1}$, $DP_p^{\boldsymbol{T}}(\boldsymbol{Q})^*(\boldsymbol{W})$ is equal to:*

$$\begin{aligned} &\left[\frac{\partial \overline{P}}{\partial x}(\star_p) - \left(-\Delta_+\frac{\partial \overline{P}}{\partial v_-}(\star)\right)_p - \left(\Delta_-\frac{\partial \overline{P}}{\partial v_+}(\star)\right)_p + \left(-\Delta_+\circ\Delta_-\frac{\partial \overline{P}}{\partial w}(\star)\right)_p\right] W_p \\ &\qquad + \left[\left(\Delta_-\frac{\partial \overline{P}}{\partial w}(\star)\right)_p - \frac{\partial \overline{P}}{\partial v_+}(\star_{p-1})\right](\Delta_-\boldsymbol{W})_p \\ &+ \left[\left(-\Delta_+\frac{\partial \overline{P}}{\partial w}(\star)\right)_p - \frac{\partial \overline{P}}{\partial v_-}(\star_{p+1})\right](-\Delta_+\boldsymbol{W})_p + \frac{\partial \overline{P}}{\partial w}(\star_p)(-\Delta_+\circ\Delta_-\boldsymbol{W})_p, \end{aligned} \tag{35}$$

where $\star := \big(\boldsymbol{Q}, \Delta_-\boldsymbol{Q}, (-\Delta_+\boldsymbol{Q}), (-\Delta_-\circ\Delta_-\boldsymbol{Q}), \boldsymbol{T}, h\big)$.

The main result of this Section is the following explicit characterization of second order finite differences operators P whose all Frechet derivatives are self-adjoint for any $\boldsymbol{T} \in \mathbb{T}$:

Theorem 11. — *Let P be a second order finite differences operator. Then, $DP^{\boldsymbol{T}}(\boldsymbol{Q})$ is self adjoint for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ if and only if P satisfies the discrete Helmholtz condition* ($\mathrm{H}_{\mathrm{disc}}$).

Proof. — Indeed, let $\boldsymbol{T} \in \mathbb{T}$ and $\boldsymbol{Q} \in \mathbb{R}^{N+1}$. According to Proposition 10, we have $DP^{\boldsymbol{T}}(\boldsymbol{Q})$ is self adjoint if and only if the right term of (34) is equal to (35) for any $\boldsymbol{W} \in \mathbb{R}^{N+1}$ and any $p = 2, ..., N-2$. Consequently, $DP^{\boldsymbol{T}}(\boldsymbol{Q})$ is self adjoint if and only for any $p = 2, ..., N-2$, the three following equalities hold:

$$\left(-\Delta_+ \circ \Delta_- \frac{\partial \overline{P}}{\partial w}(\star)\right)_p - \left(-\Delta_+ \frac{\partial \overline{P}}{\partial v_-}(\star)\right)_p - \left(\Delta_- \frac{\partial \overline{P}}{\partial v_+}(\star)\right)_p = 0, \tag{36}$$

$$\left(-\Delta_+ \frac{\partial \overline{P}}{\partial w}(\star)\right)_p - \frac{\partial \overline{P}}{\partial v_-}(\star_{p+1}) = \frac{\partial \overline{P}}{\partial v_+}(\star_p), \tag{37}$$

$$\left(\Delta_- \frac{\partial \overline{P}}{\partial w}(\star)\right)_p - \frac{\partial \overline{P}}{\partial v_+}(\star_{p-1}) = \frac{\partial \overline{P}}{\partial v_-}(\star_p), \tag{38}$$

if and only if for any $p = 2, ..., N-1$:

$$\left(\Delta_- \frac{\partial \overline{P}}{\partial w}(\star)\right)_p = \frac{\partial \overline{P}}{\partial v_-}(\star_p) + \frac{\partial \overline{P}}{\partial v_+}(\star_{p-1}). \tag{39}$$

The proof is completed. ☐

6. Proof of Theorem 5

6.1. Sufficient condition. — Let P be a second order finite differences operator associated to a second order discrete Euler-Lagrange equation. Let (L_-, L_+) denote the associated couple of Lagrangian. According to Proposition 4, we have that $\overline{P}$ satisfies (22). With a simple calculation, we can prove that for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $p = 1, ..., N-1$, the three following equalities hold:

$$\frac{\partial \overline{P}}{\partial w}(\star_p) = -\frac{\partial^2 L_-}{\partial v^2}\big(Q_{p+1}, (\Delta_- \boldsymbol{Q})_{p+1}, t_{p+1}, h\big) - \frac{\partial^2 L_+}{\partial v^2}\big(Q_{p-1}, (-\Delta_+ \boldsymbol{Q})_{p-1}, t_{p-1}, h\big), \tag{40}$$

$$\frac{\partial \overline{P}}{\partial v_-}(\star_p) = \frac{\partial^2 L_-}{\partial x \partial v}\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) - \frac{\partial^2 L_+}{\partial x \partial v}\big(Q_{p-1}, (-\Delta_+ \boldsymbol{Q})_{p-1}, t_{p-1}, h\big) + \Delta_+ \left(\frac{\partial^2 L_-}{\partial v^2}(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h)\right)_p \tag{41}$$

$$\frac{\partial \overline{P}}{\partial v_+}(\star_p) = \frac{\partial^2 L_+}{\partial x \partial v}\big(Q_p, (-\Delta_+ \boldsymbol{Q})_p, t_p, h\big) - \frac{\partial^2 L_-}{\partial x \partial v}\big(Q_{p+1}, (\Delta_- \boldsymbol{Q})_{p+1}, t_{p+1}, h\big) - \Delta_- \left(\frac{\partial^2 L_+}{\partial v^2}(\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h)\right)_p, \tag{42}$$

where $\star := \big(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, (-\Delta_+ \boldsymbol{Q}), (-\Delta_+ \circ \Delta_- \boldsymbol{Q}), \boldsymbol{T}, h\big)$. Finally, from these three equalities, we prove that P satisfies the discrete Helmholtz condition ($\mathrm{H}_{\mathrm{disc}}$).

6.2. Necessary condition. — Let P be a second order finite differences operator satisfying the discrete Helmholtz condition ($\mathrm{H}_{\mathrm{disc}}$). The proof is based on the following proposition:

Proposition 12. — *Let P be a second order finite differences operator satisfying the discrete Helmholtz condition* ($\mathrm{H}_{\mathrm{disc}}$)*. Let L_1 be the following augmented Lagrangian:*

$$\begin{array}{rrcl} L_1: & \mathbb{R}^5 \times \mathbb{R}^+_* & \longrightarrow & \mathbb{R} \\ & (x, v_-, v_+, w, t, \xi) & \longmapsto & x \displaystyle\int_0^1 \overline{P}(\lambda x, \lambda v_-, \lambda v_+, \lambda w, t, \xi)\, d\lambda \end{array} \tag{43}$$

and, for any $\boldsymbol{T} \in \mathbb{T}$, let $\mathscr{L}_1^{\boldsymbol{T}}$ denote the following augmented Lagrangian functional

$$\begin{array}{rrcl} \mathscr{L}_1^{\boldsymbol{T}}: & \mathbb{R}^{N+1} & \longrightarrow & \mathbb{R} \\ & \boldsymbol{Q} & \longmapsto & h \displaystyle\sum_{p=1}^{N-1} L_1\big(Q_p, (\Delta_- \boldsymbol{Q})_p, (-\Delta_+ \boldsymbol{Q})_p, (-\Delta_+ \circ \Delta_- \boldsymbol{Q})_p, t_p, h\big). \end{array} \tag{44}$$

Then,

1. *for any $\boldsymbol{T} \in \mathbb{T}$ and any $(\boldsymbol{Q}, \boldsymbol{W}) \in \mathbb{R}^{N+1} \times \mathbb{R}^{N+1}_{0,0}$, we have:*

$$D\mathscr{L}_1^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h \sum_{p=2}^{N-2} P_p^{\boldsymbol{T}}(\boldsymbol{Q}) W_p, \tag{45}$$

2. *there exists a couple of Lagrangian (L_-, L_+) such that for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$, we have:*

$$\begin{aligned} &L_1\big(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, (-\Delta_+ \boldsymbol{Q}), (-\Delta_- \circ \Delta_- \boldsymbol{Q}), \boldsymbol{T}, h\big) \\ &\qquad = L_-\big(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h\big) + L_+\big(\boldsymbol{Q}, (-\Delta_+ \boldsymbol{Q}), \boldsymbol{T}, h\big). \end{aligned} \tag{46}$$

Proof. — 1. Let $\boldsymbol{T} \in \mathbb{T}$ and $(\boldsymbol{Q}, \boldsymbol{W}) \in \mathbb{R}^{N+1} \times \mathbb{R}^{N+1}_{0,0}$. We have:

$$\mathscr{L}_1^{\boldsymbol{T}}(\boldsymbol{Q}) = h \sum_{p=1}^{N-1} Q_p \int_0^1 P_p^{\boldsymbol{T}}(\lambda \boldsymbol{Q})\, d\lambda. \tag{47}$$

Thus:

$$D\mathscr{L}_1^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h \sum_{p=1}^{N-1} W_p \int_0^1 P_p^{\boldsymbol{T}}(\lambda \boldsymbol{Q})\, d\lambda + h \sum_{p=1}^{N-1} Q_p \int_0^1 DP_p^{\boldsymbol{T}}(\lambda \boldsymbol{Q})(\lambda \boldsymbol{W})\, d\lambda. \tag{48}$$

As P satisfies the discrete Helmholtz condition ($\mathrm{H}_{\mathrm{disc}}$) and according to Theorem 11, $DP^{\boldsymbol{T}}(\lambda \boldsymbol{Q})$ is self-adjoint. Using Definition 8, the following equality holds:

$$h \sum_{p=1}^{N-1} DP_p^{\boldsymbol{T}}(\lambda \boldsymbol{Q})(\lambda \boldsymbol{W}) Q_p = h \sum_{p=2}^{N-2} \lambda DP_p^{\boldsymbol{T}}(\lambda \boldsymbol{Q})(\boldsymbol{Q}) W_p. \tag{49}$$

Then, from Equalities (48) and (49), we have

$$D\mathscr{L}_1^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h \sum_{p=2}^{N-2} W_p \int_0^1 P_p^{\boldsymbol{T}}(\lambda \boldsymbol{Q})\, d\lambda + h \sum_{p=2}^{N-2} W_p \int_0^1 \lambda DP_p^{\boldsymbol{T}}(\lambda \boldsymbol{Q})(\boldsymbol{Q})\, d\lambda \tag{50}$$

Then, using $\partial/\partial\lambda\big(P_p^{\boldsymbol{T}}(\lambda\boldsymbol{Q})\big) = DP_p^{\boldsymbol{T}}(\lambda\boldsymbol{Q})(\boldsymbol{Q})$ and using an integration by part with respect to λ on the second integral, we obtain:

$$D\mathcal{L}_1^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h\sum_{p=2}^{N-2} P_p^{\boldsymbol{T}}(\boldsymbol{Q})W_p. \tag{51}$$

2. Since P satisfies the discrete Helmholtz condition ($\mathrm{H}_{\mathrm{disc}}$), we have for any $\boldsymbol{T}\in\mathbb{T}$ and any $\boldsymbol{Q}\in\mathbb{R}^{N+1}$:

$$\forall p=2,...,N-1,\ \frac{1}{h}\left(\frac{\partial\overline{P}}{\partial w}(\star_p) - \frac{\partial\overline{P}}{\partial w}(\star_{p-1})\right) = \frac{\partial\overline{P}}{\partial v_-}(\star_p) + \frac{\partial\overline{P}}{\partial v_+}(\star_{p-1}), \tag{52}$$

where $\star := \big(\boldsymbol{Q},\Delta_-\boldsymbol{Q},(-\Delta_+\boldsymbol{Q}),(-\Delta_-\circ\Delta_-\boldsymbol{Q}),\boldsymbol{T},h\big)$. As it is true for any $\boldsymbol{Q}\in\mathbb{R}^{N+1}$, we can differentiate the previous equality with respect to Q_{p-2} and Q_{p+1}. It leads to the two following equalities holding for any $\boldsymbol{T}\in\mathbb{T}$, any $\boldsymbol{Q}\in\mathbb{R}^{N+1}$ and any $p=2,...,N-1$:

$$\frac{1}{h}\left(\frac{1}{h}\frac{\partial^2\overline{P}}{\partial v_-\partial w}(\star_{p-1}) - \frac{1}{h^2}\frac{\partial^2\overline{P}}{\partial w^2}(\star_{p-1})\right) = -\frac{1}{h}\frac{\partial^2\overline{P}}{\partial v_-\partial v_+}(\star_{p-1}) + \frac{1}{h^2}\frac{\partial^2\overline{P}}{\partial w\partial v_+}(\star_{p-1}) \tag{53}$$

and

$$\frac{1}{h}\left(\frac{1}{h}\frac{\partial^2\overline{P}}{\partial v_+\partial w}(\star_p) + \frac{1}{h^2}\frac{\partial^2\overline{P}}{\partial w^2}(\star_p)\right) = \frac{1}{h}\frac{\partial^2\overline{P}}{\partial v_+\partial v_-}(\star_p) + \frac{1}{h^2}\frac{\partial^2\overline{P}}{\partial w\partial v_-}(\star_p). \tag{54}$$

Finally, we have for any $\boldsymbol{T}\in\mathbb{T}$, any $\boldsymbol{Q}\in\mathbb{R}^{N+1}$ and any $p=1,...,N-1$:

$$\frac{\partial^2\overline{P}}{\partial v_+\partial v_-}(\star_p) + \frac{1}{h}\left(\frac{\partial^2\overline{P}}{\partial w\partial v_-}(\star_p) - \frac{\partial^2\overline{P}}{\partial v_+\partial w}(\star_p)\right) + \frac{1}{h^2}\frac{\partial^2\overline{P}}{\partial w^2}(\star_p) = 0. \tag{55}$$

Hence, since Equality (55) is true for any $\boldsymbol{T}\in\mathbb{T}$, any $\boldsymbol{Q}\in\mathbb{R}^{N+1}$ and any $p=1,...,N-1$, we have for any $(x,y,z,t,\xi)\in\mathbb{R}^4\times\mathbb{R}_*^+$:

$$\begin{aligned}\frac{\partial^2\overline{P}}{\partial v_+\partial v_-}\Big(x,y,z,\frac{z-y}{\xi},t,\xi\Big) + \frac{1}{h^2}\frac{\partial^2\overline{P}}{\partial w^2}\Big(x,y,z,\frac{z-y}{\xi},t,\xi\Big)&\\ + \frac{1}{h}\left(\frac{\partial^2\overline{P}}{\partial w\partial v_-}\Big(x,y,z,\frac{z-y}{\xi},t,\xi\Big) - \frac{\partial^2\overline{P}}{\partial v_+\partial w}\Big(x,y,z,\frac{z-y}{\xi},t,\xi\Big)\right) &= 0.\end{aligned} \tag{56}$$

Let us define:

$$\begin{array}{rccl}\ell: & \mathbb{R}^4\times\mathbb{R}_*^+ & \longrightarrow & \mathbb{R}\\ & (x,y,z,t,\xi) & \longmapsto & \overline{P}\Big(x,y,z,\dfrac{z-y}{\xi},t,\xi\Big).\end{array} \tag{57}$$

According to (56), we have:

$$\forall(x,y,z,t,\xi)\in\mathbb{R}^4\times\mathbb{R}_*^+,\ \frac{\partial^2\ell}{\partial z\partial y}(x,y,z,t,\xi) = 0. \tag{58}$$

Consequently, the variables y and z are separable in ℓ. Precisely, there exist two functions $\alpha,\ \beta:\mathbb{R}^3\times\mathbb{R}_*^+\longrightarrow\mathbb{R}$ such that:

$$\forall(x,y,z,t,\xi)\in\mathbb{R}^4\times\mathbb{R}_*^+,\ \ell(x,y,z,t,\xi) = \alpha(x,y,t,\xi) + \beta(x,z,t,\xi). \tag{59}$$

Finally, we have for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $p = 1, ..., N-1$:

$$\begin{aligned} L_1(\star_p) &= Q_p \left(\int_0^1 \overline{P}\big(\lambda Q_p, \lambda(\Delta_- \boldsymbol{Q})_p, \lambda(-\Delta_+ \boldsymbol{Q})_p, \lambda(-\Delta_+ \circ \Delta_- \boldsymbol{Q})_p, t_p, h\big)\, d\lambda \right) && (60) \\ &= Q_p \left(\int_0^1 \ell\big(\lambda Q_p, \lambda(\Delta_- \boldsymbol{Q})_p, \lambda(-\Delta_+ \boldsymbol{Q})_p, t_p, h\big)\, d\lambda \right) && (61) \\ &= Q_p \left(\int_0^1 \alpha\big(\lambda Q_p, \lambda(\Delta_- \boldsymbol{Q})_p, t_p, h\big) + \beta\big(\lambda Q_p, \lambda(-\Delta_+ \boldsymbol{Q})_p, t_p, h\big)\, d\lambda \right) && (62) \\ &= L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + L_+\big(Q_p, (-\Delta_+ \boldsymbol{Q})_p, t_p, h\big), && (63) \end{aligned}$$

where:

$$\begin{aligned} L_- : \quad \mathbb{R}^3 \times \mathbb{R}^+_* &\longrightarrow \mathbb{R} && (64) \\ (x, v, t, \xi) &\longmapsto x \int_0^1 \alpha(\lambda x, \lambda v, t, \xi)\, d\lambda \end{aligned}$$

and

$$\begin{aligned} L_+ : \quad \mathbb{R}^3 \times \mathbb{R}^+_* &\longrightarrow \mathbb{R} && (65) \\ (x, v, t, \xi) &\longmapsto x \int_0^1 \beta(\lambda x, \lambda v, t, \xi)\, d\lambda. \end{aligned}$$

The proof of Proposition 12 is now completed. □

Now, from Proposition 12, we are going to prove Theorem 5. Precisely, let us define, for any $\boldsymbol{T} \in \mathbb{T}$, the following discrete Lagrangian functional:

$$\begin{aligned} \mathscr{L}^{\boldsymbol{T}} : \quad \mathbb{R}^{N+1} &\longrightarrow \mathbb{R} && (66) \\ \boldsymbol{Q} &\longmapsto h \sum_{p=1}^{N} L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + h \sum_{p=0}^{N-1} L_+\big(Q_p, (-\Delta_+ \boldsymbol{Q})_p, t_p, h\big) \end{aligned}$$

where (L_-, L_+) is the couple of Lagrangian given in the point 2 of Proposition 12. Then, we have for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$:

$$\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q}) = \mathscr{L}_1^{\boldsymbol{T}}(\boldsymbol{Q}) + hL_- \left(Q_N, \frac{Q_N - Q_{N-1}}{h}, t_N, h \right) + hL_+ \left(Q_0, \frac{Q_1 - Q_0}{h}, t_0, h \right), \quad (67)$$

where $\mathscr{L}_1^{\boldsymbol{T}}$ is defined in Proposition 12. Consequently, we have for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $\boldsymbol{W} \in \mathbb{R}^{N+1}_{0,0}$:

$$D\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = D\mathscr{L}_1^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h \sum_{p=2}^{N-2} P_p^{\boldsymbol{T}}(\boldsymbol{Q}) W_p. \quad (68)$$

However, using the same method than in the proof of Theorem 3, we prove from Equation (66) that for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $\boldsymbol{W} \in \mathbb{R}^{N+1}_{0,0}$:

$$D\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = h \sum_{p=2}^{N-2} \left[\frac{\partial L_-}{\partial x}(*_p) + \frac{\partial L_+}{\partial x}(**_p) + \Delta_+ \left(\frac{\partial L_-}{\partial v}(*) \right)_p - \Delta_- \left(\frac{\partial L_+}{\partial v}(**) \right)_p \right] W_p, \quad (69)$$

where $* := (\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h)$ and $** := (\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h)$. Combining Equalities (68) and (69), we conclude that for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $p = 2, ..., N-2$:

$$P_p^{\boldsymbol{T}}(\boldsymbol{Q}) = \frac{\partial L_-}{\partial x}(*_p) + \frac{\partial L_+}{\partial x}(**_p) + \Delta_+ \left(\frac{\partial L_-}{\partial v}(*) \right)_p - \Delta_- \left(\frac{\partial L_+}{\partial v}(**) \right)_p . \tag{70}$$

In order to finish the proof of Theorem 5, we have just to prove that Equality (70) is still true for $p = 1$ and $p = N-1$. We only prove it for $p = N-1$. The case $p = 1$ can be proved in a similar way.

In this way, let us take $\boldsymbol{T} \in \mathbb{T}$ and $\boldsymbol{Q} \in \mathbb{R}^{N+1}$. Let us denote $\sigma(\boldsymbol{T}) = (t_{p+1})_{p=0,...,N} \in \mathbb{T}$ and $\sigma(\boldsymbol{Q}) = (Q_{p+1})_{p=0,...,N} \in \mathbb{R}^{N+1}$ where $t_{N+1} := t_N + h$ and $Q_{N+1} := 0$. From Equality (70), we have:

$$\begin{aligned} P_{N-1}^{\boldsymbol{T}}\big(\boldsymbol{Q}\big) = P_{N-2}^{\sigma(\boldsymbol{T})}\big(\sigma(\boldsymbol{Q})\big) = \frac{\partial L_-}{\partial x}\big(\sigma(*)_{N-2}\big) + \frac{\partial L_+}{\partial x}\big(\sigma(**)_{N-2}\big) \\ + \Delta_+ \left(\frac{\partial L_-}{\partial v}\big(\sigma(*)\big) \right)_{N-2} - \Delta_- \left(\frac{\partial L_+}{\partial v}\big(\sigma(**)\big) \right)_{N-2}, \end{aligned} \tag{71}$$

where $\sigma(*) := \big(\sigma(\boldsymbol{Q}), \Delta_- \sigma(\boldsymbol{Q}), \sigma(\boldsymbol{T}), h\big)$ and $\sigma(**) := \big(\sigma(\boldsymbol{Q}), -\Delta_+ \sigma(\boldsymbol{Q}), \sigma(\boldsymbol{T}), h\big)$. Consequently, we have:

$$P_{N-1}^{\boldsymbol{T}}\big(\boldsymbol{Q}\big) = \frac{\partial L_-}{\partial x}(*_{N-1}) + \frac{\partial L_+}{\partial x}(**_{N-1}) + \Delta_+ \left(\frac{\partial L_-}{\partial v}(*) \right)_{N-1} - \Delta_- \left(\frac{\partial L_+}{\partial v}(**) \right)_{N-1} . \tag{72}$$

The proof of Theorem 5 is completed.

7. Characterization of the null (couples of) Lagrangian

In this section, we are interested in the second part of the Helmholtz problem both in the continuous and discrete cases. Precisely, once the Helmholtz condition satisfied, can we characterize all the possible (couple of) Lagrangian leading to the same second order (discrete) Euler-Lagrange equation?

7.1. Reminder of the continuous case. — Let L^1, L^2 be two Lagrangian. They are said to be *equivalent* if they lead to the same second order Euler-Lagrange equation. In this case, we denote $L^1 \sim L^2$. The linearity of the Euler-Lagrange equation with respect to its associated Lagrangian implies that $\sim$ defines an equivalence relation on the set of Lagrangian.

Hence, the aim is to characterize the equivalence class of 0. If a Lagrangian L belongs to the equivalence class of 0, then it it leads to a null second order Euler-Lagrange equation in the sense that every curves q are solutions. In this case, L is said to be a *null Lagrangian*. We refer to [**13**] for a detailed proof of the following result:

Theorem 13. — *Let L be a Lagrangian. L is a null Lagrangian if and only if there exist two functions $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ and $g : \mathbb{R} \longrightarrow \mathbb{R}$ such that:*

$$\forall a < b,\ \forall q \in \mathscr{C}^2([a,b], \mathbb{R}),\ L(q, \dot{q}, t) = \frac{d}{dt}\big(f(q,t)\big) + g(t). \tag{73}$$

Let us note that, in the major of literature, the previous theorem is presented with $g = 0$. Indeed, we have just to add an anti-derivative of g to f. However, in the next section, we can prove the discrete version of Theorem 13 only with this presentation.

7.2. The discrete case. — In the discrete case, we give the following discrete versions of the definitions and results of the previous section.

Definition 14. — *Let (L^1_-, L^1_+) and (L^2_-, L^2_+) be two couples of Lagrangian. We say that they are equivalent if they lead to the same discrete second order Euler-Lagrange equation* $(\mathrm{EL}^{\boldsymbol{T}})$. *In this case, we denote $(L^1_-, L^1_+) \sim (L^2_-, L^2_+)$. The linearity of the discrete Euler-Lagrange equation with respect to its associated couple of Lagrangian implies that $\sim$ defines an equivalence relation on the set of couple of Lagrangian. If a couple of Lagrangian (L_-, L_+) belongs to the equivalence class of 0, then it leads to a null second order discrete Euler-Lagrange equation in the sense that every discrete curves $\boldsymbol{Q}$ are solutions. In this case, (L_-, L_+) is said to be a null couple of Lagrangian.*

Our aim is then to characterize the set of the null couple of Lagrangian. It is done in the following result:

Theorem 15. — *Let (L_-, L_+) be a couple of Lagrangian. (L_-, L_+) is a null couple of Lagrangian if and only if there exist two functions $f : \mathbb{R}^2 \times \mathbb{R}^+_* \longrightarrow \mathbb{R}$ and $g : \mathbb{R} \times \mathbb{R}^+_* \longrightarrow \mathbb{R}$ such that for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $p = 1, ..., N$:*

$$L_-\big(Q_p, (\Delta_- Q)_p, t_p, h\big) + L_+\big(Q_{p-1}, (-\Delta_+ Q)_{p-1}, t_{p-1}, h\big) = \Delta_-\big(f(\boldsymbol{Q}, \boldsymbol{T}, h)\big)_p + g(t_p, h). \tag{74}$$

Proof. — Let us prove the sufficient condition. Let us assume that Equation (74) is true and let $\mathscr{L}^{\boldsymbol{T}}$ denote the discrete Lagrangian functional associated to (L_-, L_+) and to a partition $\boldsymbol{T} \in \mathbb{T}$. Then, we have for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$:

$$\begin{aligned}
\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q}) &= h \sum_{p=1}^{N} L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + h \sum_{p=0}^{N-1} L_+\big(Q_p, (-\Delta_+ \boldsymbol{Q})_p, t_p, h\big) \\
&= h \sum_{p=1}^{N} \Big[L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + L_+\big(Q_{p-1}, (-\Delta_+ Q)_{p-1}, t_{p-1}, h\big)\Big] \\
&= h \sum_{p=1}^{N} \Big[\Delta_-\big(f(\boldsymbol{Q}, \boldsymbol{T}, h)\big)_p + g(t_p, h)\Big] \\
&= f(Q_N, t_N, h) - f(Q_0, t_0, h) + h \sum_{p=1}^{N} g(t_p, h).
\end{aligned}$$

Consequently, since the set of discrete variations is $\mathbb{R}^{N+1}_0$, every discrete curves $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ are discrete critical points of $\mathscr{L}^{\boldsymbol{T}}$ and then the discrete Euler-Lagrange equation associated is null. Then, (L_-, L_+) is a null couple of Lagrangian.

Now, let us prove the necessary condition. Let us assume that (L_-, L_+) is a null couple of Lagrangian. Then, for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$, we have:

$$\frac{\partial L_-}{\partial x}(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h) + \frac{\partial L_+}{\partial x}(\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h) \\ + \Delta_+ \left(\frac{\partial L_-}{\partial v}(\boldsymbol{Q}, \Delta_- \boldsymbol{Q}, \boldsymbol{T}, h) \right) - \Delta_- \left(\frac{\partial L_+}{\partial v}(\boldsymbol{Q}, -\Delta_+ \boldsymbol{Q}, \boldsymbol{T}, h) \right) = 0. \quad (75)$$

Then, let us define:

$$\begin{array}{rccc} \ell_- : & \mathbb{R}^3 \times \mathbb{R}^+_* & \longrightarrow & \mathbb{R} \\ & (x_1, x_2, t, \xi) & \longmapsto & L_-\Big(x_1, \dfrac{x_1 - x_2}{\xi}, t, \xi\Big) \end{array} \quad (76)$$

and

$$\begin{array}{rccc} \ell_+ : & \mathbb{R}^3 \times \mathbb{R}^+_* & \longrightarrow & \mathbb{R} \\ & (x_1, x_2, t, \xi) & \longmapsto & L_+\Big(x_1, \dfrac{x_2 - x_1}{\xi}, t, \xi\Big). \end{array} \quad (77)$$

Since Equality (75) is true for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$, we have for any $(x, y, z, t, \xi) \in \mathbb{R}^4 \times \mathbb{R}^+_*$:

$$\frac{\partial \ell_-}{\partial x_1}(x, y, t, \xi) + \frac{\partial \ell_-}{\partial x_2}(z, x, t + \xi, \xi) + \frac{\partial \ell_+}{\partial x_1}(x, z, t, \xi) + \frac{\partial \ell_+}{\partial x_2}(y, x, t - \xi, \xi) = 0. \quad (78)$$

Then, by differentiating the previous equality with respect to y or to z, we obtain for any $(x, y, t, \xi) \in \mathbb{R}^3 \times \mathbb{R}^+_*$:

$$\frac{\partial^2 \ell_-}{\partial x_1 \partial x_2}(x, y, t, \xi) + \frac{\partial^2 \ell_+}{\partial x_1 \partial x_2}(y, x, t - \xi, \xi) = 0. \quad (79)$$

Consequently, there exist two functions $\alpha, \beta : \mathbb{R}^2 \times \mathbb{R}^+_* \longrightarrow \mathbb{R}$ such that for any $(x, y, t, \xi) \in \mathbb{R}^3 \times \mathbb{R}^+_*$:

$$\ell_-(x, y, t, \xi) + \ell_+(y, x, t - \xi, \xi) = \alpha(x, t, \xi) + \beta(y, t, \xi). \quad (80)$$

Moreover, let us denote $\mathscr{L}^{\boldsymbol{T}}$ the discrete Lagrangian functional associated to (L_-, L_+) and to a partition $\boldsymbol{T} \in \mathbb{T}$. Then, we have for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$:

$$\begin{aligned} \mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q}) &= h \sum_{p=1}^{N} L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + h \sum_{p=0}^{N-1} L_+\big(Q_p, (-\Delta_+ \boldsymbol{Q})_p, t_p, h\big) \\ &= h \sum_{p=1}^{N} \Big[L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + L_+\big(Q_{p-1}, (-\Delta_+ Q)_{p-1}, t_{p-1}, h\big) \Big] \\ &= h \sum_{p=1}^{N} \Big[\ell_-(Q_p, Q_{p-1}, t_p, h) + \ell_+(Q_{p-1}, Q_p, t_{p-1}, h) \Big] \\ &= h \sum_{p=1}^{N} \Big[\alpha(Q_p, t_p, h) + \beta(Q_{p-1}, t_p, h) \Big]. \end{aligned}$$

With a discrete calculus of variations, we obtain for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $\boldsymbol{W} \in \mathbb{R}_0^{N+1}$:

$$D\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = \sum_{p=1}^{N-1} \Big[\frac{\partial \alpha}{\partial x_1}(Q_p, t_p, h) + \frac{\partial \beta}{\partial x_1}(Q_p, t_{p+1}, h) \Big] W_p. \tag{81}$$

Since (L_-, L_+) is a null couple of Lagrangian, we have $D\mathscr{L}^{\boldsymbol{T}}(\boldsymbol{Q})(\boldsymbol{W}) = 0$ for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $\boldsymbol{W} \in \mathbb{R}_0^{N+1}$. Consequently, for any $\boldsymbol{T} \in \mathbb{T}$ and any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$, we have:

$$\frac{\partial \alpha}{\partial x_1}(Q_p, t_p, h) + \frac{\partial \beta}{\partial x_1}(Q_p, t_{p+1}, h) = 0. \tag{82}$$

Consequently, we have for any $(x, t, \xi) \in \mathbb{R}^2 \times \mathbb{R}_*^+$:

$$\frac{\partial \alpha}{\partial x_1}(x, t, \xi) + \frac{\partial \beta}{\partial x_1}(x, t+\xi, \xi) = 0. \tag{83}$$

Hence, there exists a function $\gamma : \mathbb{R} \times \mathbb{R}_*^+ \longrightarrow \mathbb{R}$ such that:

$$\forall (x, t, \xi) \in \mathbb{R}^2 \times \mathbb{R}_*^+, \ \alpha(x, t, \xi) + \beta(x, t+\xi, \xi) = \gamma(t, \xi). \tag{84}$$

Then, according to Equality (80), we have for any $(x, y, t, \xi) \in \mathbb{R}^3 \times \mathbb{R}_*^+$:

$$\ell_-(x, y, t, \xi) + \ell_+(y, x, t-\xi, \xi) = \alpha(x, t, \xi) - \alpha(y, t-\xi, \xi) + \gamma(t-\xi, \xi). \tag{85}$$

Thus, we have for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $p = 1, ..., N$:

$$\begin{aligned} L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + L_+\big(Q_{p-1}, (-\Delta_+ Q)_{p-1}, t_{p-1}, h\big) & \\ = \ \ell_-(Q_p, Q_{p-1}, t_p, h) + \ell_+(Q_{p-1}, Q_p, t_{p-1}, h) & \\ = \ \alpha(Q_p, t_p, h) - \alpha(Q_{p-1}, t_{p-1}, h) + \gamma(t_{p-1}, h) & \end{aligned} \tag{86}$$

Hence, let us define:

$$\begin{array}{rccc} f: & \mathbb{R}^2 \times \mathbb{R}_*^+ & \longrightarrow & \mathbb{R} \\ & (x, t, \xi) & \longmapsto & \xi \alpha(x, t, \xi) \end{array} \tag{87}$$

and

$$\begin{array}{rccc} g: & \mathbb{R} \times \mathbb{R}_*^+ & \longrightarrow & \mathbb{R} \\ & (t, \xi) & \longmapsto & \gamma(t-\xi, \xi). \end{array} \tag{88}$$

Then, we have for any $\boldsymbol{T} \in \mathbb{T}$, any $\boldsymbol{Q} \in \mathbb{R}^{N+1}$ and any $p = 1, ..., N$:

$$L_-\big(Q_p, (\Delta_- \boldsymbol{Q})_p, t_p, h\big) + L_+\big(Q_{p-1}, (-\Delta_+ Q)_{p-1}, t_{p-1}, h\big) = \Delta_-\big(f(\boldsymbol{Q}, \boldsymbol{T}, h)\big)_p + g(t_p, h). \tag{89}$$

The proof is completed. □

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